The Ehrenfest system and the rest point spectrum for a Hartree-type Equation

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Abstract. Following Ehrenfest's approach, the problem of quantum-classical correspondence can be treated in the class of trajectory-coherent functions that approximate as $\hbar \to 0$ a quantum-mechanical state. This idea leads to a family of systems of ordinary differential equations, called Ehrenfest M-systems ($M = 0, 1, 2, \dots$), formally equivalent to the semiclassical approximation for the linear Schrödinger equation [16, 22].

In this paper a similar approach is undertaken for a nonlinear Hartree-type equation with a smooth integral kernel. It is demonstrated how quantum characteristics can be retrieved directly from the corresponding Ehrenfest systems, without solving the quantum equation: the semiclassical asymptotics for the spectrum are obtained from the rest point solution. One of the key steps is derivation of a modified nonlinear superposition principle valid in the class of trajectory-coherent quantum states.

Introduction

Semiclassical methods play a distinguished role among asymptotic approaches in linear mathematical physics. From the very beginning of quantum mechanics semiclassical approximation has been one of the the main technical tools to address its two aspects: pragmatic and philosophical.

The pragmatic (computational) aspect relies on the presence of a *small* parameter $\hbar$ as a factor next to the derivatives. The pattern is demonstrated in the Schrödinger evolution equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{\mathcal{H}}\Psi, \qquad \hat{\mathcal{H}} = \frac{\hat{\vec{p}}^{\,2}}{2m} + U(\vec{x}), \quad \hat{\vec{p}} = -i\hbar\nabla_x, \quad \vec{x} \in \mathbb{R}^n, \tag{0.1}$$

corresponding to the classical Hamilton function

$$\mathcal{H}(\vec{p}, \vec{x}, t) = \frac{\vec{p}^{\,2}}{2m} + U(\vec{x}). \tag{0.2}$$

While Planck's $\hbar$ is a dimensional constant, there exists a large class of quantum-mechanical problems where a small dimensionless parameter, proportional to $\hbar$, is present. Accordingly, there is a mathematical problem to construct an approximate (with respect to that parameter) solution of the quantum mechanical equation. Such an approximate solution is traditionally termed *the semiclassical asymptotics as* $\hbar \to 0$.

The philosophical aspect is related to the correspondence principle, one of the cornerstones of quantum mechanics. Despite the fact that quantum mechanics in its axiomatic formalization is a self-consistent theory and does not appeal to the classical mechanics, the correspondence principle requires the classical equations of motion to emerge from the quantum theory in the limit $\hbar \to 0$.

Obviously, there is no universal (i.e. physical problem independent) way to obtain arbitrary classical values from quantum-mechanical values. In each particular case it is necessary to specify in what sense a quantum characteristic becomes classical as $\hbar \to 0$. The problem of deriving classical equations of motion from those of quantum mechanics in the limit $\hbar \to 0$ is one of the principal questions of the quantum-classical correspondence.

Historically, there are a number of approaches to the problem. One of them is due to Born [1], in which a quantum system is approximately described by the classical statistical ensemble expressed

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via a semiclassical wave function. A justification of this approach is based on the construction of a semiclassical solution to the quantum equation. The time-global version of such a construction is known as the Maslov canonical operator [2, 3]. In this approach the correspondence principle reveals itself in the fact that the principal term of the asymptotic expansion of the quantum density matrix is a solution of the classical Liouville equation.

Another approach, suggested by Ehrenfest [4], is based on the idea that Newtonian equations of motion can be obtained in the limit $\hbar \to 0$ from equations for mean values of the corresponding quantum-mechanical observables. More generally, any ordinary differential equations (ODE) obtained in the same manner from equations of quantum mechanics can be called classical. The correspondence between a quantum observable and its classical counterpart (assuming that such exists) is understood as follows: the quantum mean value $\langle \hat{A} \rangle_\Psi$ of the observable $\hat{A} = A(\hat{z}, \hbar)$ calculated with respect to some special non-stationary states $\Psi(t; \hbar)$ must yield in the limit $\hbar \to 0$ the corresponding classical observable A evaluated on a certain classical trajectory $z(t)$ in the phase space

$$\lim_{\hbar \to 0} \langle \hat{A} \rangle_\Psi = A(z(t), 0). \tag{0.3}$$

For the Schrödinger equation (0.1) the Ehrenfest approach relies on states $\Psi(\vec{x}, t; \hbar)$ that are *localized on the classical trajectory* in the following sense: the mean values

$$\bar{x}_k(t, \hbar) \equiv \langle \hat{x}_k \rangle_\Psi = \int_{\mathbb{R}^n} x_k |\Psi|^2 d\vec{x}, \quad \bar{p}_k(t, \hbar) \equiv \langle \hat{p}_k \rangle_\Psi = \int_{\mathbb{R}^n} \Psi^* \hat{p}_k \Psi d\vec{x}, \qquad k = \overline{1, n}, \tag{0.4}$$

of the operators of coordinates $\hat{\vec{x}} = (x_1, \dots, x_n)$ and momenta $\hat{\vec{p}} = -i\hbar\nabla$ calculated with respect to such states $\Psi(x, t; \hbar)$ in the limit $\hbar \to 0$

$$X_k(t) = \lim_{h \to 0} \bar{x}_k(t, \hbar), \quad P_k(t) = \lim_{h \to 0} \bar{p}_k(t, \hbar), \qquad k = \overline{1, n}, \tag{0.5}$$

obey the classical Hamiltonian system

$$m\dot{\vec{X}} = \vec{P}, \quad \dot{\vec{P}} = -\nabla_x U(\vec{X}). \tag{0.6}$$

A function Ψ for which the limits (0.5) exist was called in [5, 6] a *trajectory-coherent state*.

The technical implementation of the Ehrenfest approach is based on the construction of either exact or approximate trajectory-coherent solutions of the Schrödinger equation. Exact trajectory-coherent solutions are available only for special Hamiltonians, such as (0.1) with quadratic potential. Examples are well-known coherent and squeezed coherent states [7, 8]. An approximate ($\hbar \to 0$) trajectory-coherent solution, called a *semiclassically concentrated state* can be constructed in a much wider class of problems, employing the ideas of the complex WKB-Maslov method [9,10] (see also [11–14]). The correspondence principle is manifested in this construction: a trajectory-coherent state is an approximate ($\hbar \to 0$) solution of (0.1) (i.e. it is a semiclassically concentrated state) if and only if the trajectory (0.5) satisfies the classical equation (0.6). The semiclassically concentrated states were first found for particles moving in a potential field [15], and later in an arbitrary electromagnetic field [5, 6]. Detailed bibliography can be found in the reviews [14, 16].

It was found that semiclassically concentrated states exist for linear equations of quantum mechanics describing a charged particle with spin or isospin in an external field. In [17–21] the semiclassically concentrated states were constructed for the Klein-Gordon and Dirac-Pauli equations in an arbitrary electromagnetic field as well as for the Schrödinger and Dirac equations in an arbitrary non-abelian field with gauge group $SU(2)$.

The existence of the semiclassically concentrated states is essential for the approach employed in this paper, which consists of the following. Consider an observable $\hat{A} = A(\hat{z})$ whose classical analog is $A(z)$. Its mean value in a semiclassically concentrated state can be expressed to any accuracy $O(\hbar^{(M+1)/2})$ via a solution $\{z(t), \Delta^2(t), \dots, \Delta^M(t)\}$ of a finite system of ODEs ,

$$\langle \hat{A} \rangle_\Psi = A(z(t)) + \sum_{k=2}^{M} A_k(z(t)) \cdot \Delta^k(t) + O(\hbar^{(M+1)/2}), \qquad \Delta^k(t) = O(\hbar^{k/2}), \tag{0.7}$$

where tensors $A_k(z)$ comprise all partial derivatives of A of order k at the point z, and tensors Δ^k comprise all moments of order k (see (0.9) below).

The dimension of the ODE system is determined by the order of accuracy M. For instance, if $M = 0$ or 1 (it appears that $\Delta^1 = 0$ by construction), we obtain

$$\langle \hat{A} \rangle_\Psi = A(z(t)) + O(\hbar),$$

where $z(t)$ is subject to classical-mechanics equations, in accordance to Ehrenfest's original idea (0.3). In our approach, by classical equations (of order $M \geqslant 0$) corresponding to a quantum equation we mean that finite system of ODEs whose solution provides accuracy $O(\hbar^{(M+1)/2})$ in (0.7), and we call it the *Ehrenfest M-system*.

The Ehrenfest systems of finite order are truncations of an infinite ODE system, which describes evolution of the mean values for a basic infinite set of observables. For the Schrödinger equation (0.1) the basic set consists of $\hat{\vec{x}}$, $\hat{\vec{p}}$ and a special basis of the universal enveloping of the Heisenberg-Weyl algebra with generators $\hat{I}$, $\Delta\hat{x}_k = \hat{x}_k - \bar{x}_k(t)$, $\Delta\hat{p}_k = \hat{p_k} - \bar{p}_k$, $1 \leqslant k \leqslant n$, where $\hat{I}$ is the identity operator and $\bar{x}_k$, $\bar{p}_k$ are defined in (0.4). The truncations leading to M-systems are made due to the estimates for Δ^k in (0.7), which allow to disregard within given accuracy $O(\hbar^{(M+1)/2})$ all variables Δ^k for $k > M$ when the means are calculated with respect to semiclassically-concentrated states. The $M = 0$ truncation is simply Newton's system (0.6); similarly, the Ehrenfest 0-system for the Klein-Gordon equation is the Lorentz equation.

The infinite ODE system for (0.1) was derived in [22–24] and it was called the Hamilton-Ehrenfest system in [16]. The name reflects a non-trivial fact that the infinite system can be written in the Hamiltonian form with respect to a degenerate nonlinear Dirac bracket [25]. A system with similar algebraic structure was also derived for the (matrix) Pauli equation [26]. A Hamiltonian structure with a degenerate Poisson bracket is also known for the $M = 2$ truncation [25, 27, 28]. The truncated systems were independently introduced in [29] and used to study quantum problems with underlying classically chaotic dynamics.

In a number of examples this approach was shown to agree with known "classical" equations of motion even in the cases where no corresponding classical observables existed. For the Dirac-Pauli equation in an external field the Ehrenfest 0-system is a pair of classical equations which are the Lorentz equation and the Bargmann-Michel-Telegdi [30] equation in which the field is calculated on the trajectories of the Lorentz equation. The order $M = 2$ truncation obtained in [21] is a Frenkel type [31] ODE for spin motion. For the Schrödinger and Dirac equations in external fields with gauge group $SU(2)$ the Ehrenfest 2-system [18,20] yields the Wong [32] equation for a non-abelian particle with isospin 1/2. More examples of derivations of known "classical" equations from the Dirac equation with external fields and the Prock equation are given in [33–35].

The Ehrenfest M-system is semiclassically equivalent with accuracy $O(\hbar^{(M+1)/2})$ to the Schrödinger equation in the class of trajectory-concentrated states in the sense that it allows us to calculate the mean value of an observable directly from the solutions of the system. An explicit formula for the state is not required. It was also observed that under certain conditions one can obtain asymptotics for pure quantum characteristics, such as energy spectrum series, from stationary or periodic solutions of the Ehrenfest 2-system.

The goal of this paper is to generalize the approach for the case of a nonlinear Hartree-type equation. In particular, we consider the following equation of self-consistent field

$$\begin{aligned} &i\hbar\frac{\partial\Psi}{\partial t} = \widehat{\mathcal{H}}_{\varkappa}(\Psi)\Psi, \\ &\widehat{\mathcal{H}}_{\varkappa}(\Psi) = -\frac{\hbar^2}{2m}\nabla_x^2 + U(\vec{x}) + \varkappa\int\limits_{\mathbb{R}^n} V(\vec{x},\vec{y})\big|\Psi(\vec{y},t)\big|^2\,d\vec{y}, \qquad \vec{x}\in\mathbb{R}^n, \end{aligned} \tag{0.8}$$

where $U(\vec{x})$ and $V(\vec{x},\vec{y})$ are given smooth potentials of the external electromagnetic field and the self-consistent field respectively, and $\varkappa$ is a constant.

There are at least two reasons why the problem of quantum-classical correspondence was not considered in the spirit of Ehrenfest's approach, neither for a nonlinear self-consistent field (0.8), nor for more general Hartree-type equations.

First, the operator $\widehat{\mathcal{H}}_{\varkappa}(\Psi)$ does not have a natural classical analog in the traditional sense, thus it is not *a priori* obvious which dynamical Ψ-independent system is an appropriate candidate for the "classical" system in the limit $\hbar \to 0$.

Second, it is not clear whether the nonlinear quantum equation has either exact or approximate (as $\hbar \to 0$) solutions that are trajectory-coherent in the sense of (0.5).

In the framework of our approach, a solution of the correspondence problem includes three stages.

1. First, for an arbitrary one parameter family of phase space trajectories $Z(t,\hbar) = (\vec{P}(t,\hbar), \vec{X}(t,\hbar))$, $t \in \mathbb{R}$, we introduce a class $\mathcal{P}_\hbar^t(Z(t,\hbar))$ of *trajectory-coherent functions*. Exact construction is given in Sect. 2.

   Let $\alpha, \beta \in \mathbb{Z}_+^n$ be multi-indices, $|\alpha| = \sum_{k=1}^n \alpha_k$, and $\vec{X}^\alpha = \prod_{j=1}^n X_j^{\alpha_j}$. Let $\widehat{\Delta}_{\alpha\beta}$ be an operator with Weyl symbol $\Delta_{\alpha\beta}(\vec{p},\vec{x}) = \big(\vec{x} - \vec{X}(t)\big)^\alpha\big(\vec{p} - \vec{P}(t)\big)^\beta$. The following property is essential for

further steps: the centered moments

$$\Delta_{\alpha\beta}(t,\hbar) = \left\langle \widehat{\Delta}_{\alpha\beta} \right\rangle_{\Psi}, \tag{0.9}$$

calculated with respect to functions from class $\mathcal{P}_\hbar^t(Z(t,\hbar))$ satisfy the estimate

$$\Delta_{\alpha\beta} = O\Big(\hbar^{(|\alpha|+|\beta|)/2}\Big), \quad \hbar \to 0.$$

Consequently, k-th order moments (i.e. those with $|\alpha|+|\beta| = k$) are $O(\hbar^{k/2})$.

2. Next, we assume that equation (0.8) has either an exact or approximate (with accuracy $O(h^{(M+1)/2})$, $M \geqslant 0$) solution Ψ in the class of trajectory-coherent functions. Using an approach similar to the linear case, we derive an infinite Ehrenfest system for the nonlinear equation (0.8) and its finite M-truncations for $\{\big(\vec{P}(t,\hbar), \vec{X}(t,\hbar)\big),\ \Delta_{\alpha\beta}(t,\hbar), \quad |\alpha|+|\beta| \leqslant M\}$. Details are provided in Sect. 3. In particular, the principal ($M = 0$) Ehrenfest system for the nonlinear equation of self-consistent field has the form

$$\begin{aligned} &m\dot{\vec{X}} = \vec{P}, \\ &\dot{\vec{P}} = -\nabla_x U(\vec{X}) - \varkappa \nabla_x V(\vec{x},\vec{y})\Big|_{\vec{y}=\vec{x}=\vec{X}}. \end{aligned} \tag{0.10}$$

Note that when $\varkappa = 0$, this system turns to (0.6). Similarly to the latter, the system (0.10) describes $\mod \hbar^{1/2}$ the trajectory where the trajectory-coherent solution $\Psi \in \mathcal{P}_\hbar^t$ is localized.

3. Given a semiclassically-concentrated solution of equation (0.8) with accuracy $O(\hbar^{(M+1)/2})$, one can obtain a corresponding solution to the Ehrenfest system of order M by evaluating mean values of operators $\hat{\vec{x}}$, $\hat{\vec{p}}$, $\widehat{\Delta}_{\alpha\beta}$ with respect to that solution. Our goal is to show that it works the other way around as well: quantum characteristics can be found with accuracy $O(\hbar^{(M+1)/2})$ from a solution of the Ehrenfest M-system.

   In Section 4 we study the Ehrenfest 2-system for the Hartree-type equation and in particular its solutions corresponding to the rest point of the classical ($M = 0$) system. Based on this calculation, in Section 5 we reconstruct the asymptotics of the energy spectrum for the Hartree-type equation. Examples in Section 6 illustrate general results.

The key point of the whole approach is to obtain quantum characteristics without explicitly solving the quantum mechanical equation. An explicit formula for the solutions is not required anywhere in the derivation. A basic assumption of the paper is the existence of a semiclassically concentrated solution of the Hartree-type equation in a class $\mathcal{P}_\hbar^t$. This assumption can be justified by explicit construction of formal asymptotic solutions using finite dimensional Ehrenfest systems [36–40].

1. Hartree-type equation

By the Hartree-type equation we mean the following equation

$$\{-i\hbar\partial_t + \hat{\mathcal{H}}_\varkappa(\Psi)\}\Psi = 0, \qquad \hat{\mathcal{H}}_\varkappa(\Psi) = \hat{\mathcal{H}} + \varkappa\hat{V}(\Psi), \quad \Psi \in L_2(\mathbb{R}^n_x). \tag{1.1}$$

Here

$$\hat{\mathcal{H}} = \mathcal{H}(\hat{z}), \quad \hat{V}(\Psi) = \int\limits_{\mathbb{R}^n} d\vec{y}\, \Psi^*(\vec{y},t) V(\hat{z},\hat{w})\Psi(\vec{y},t), \tag{1.2}$$

where the pseudo-differential operators $\mathcal{H}(\hat{z})$ and $V(\hat{z},\hat{w})$ with symbols $\mathcal{H}(z)$ and $V(z,w)$ respectively are functions of non-commutative operators

$$\hat{z} = (-i\hbar\nabla_x, \vec{x}), \qquad \hat{w} = (-i\hbar\nabla_y, \vec{y}), \qquad \vec{x},\vec{y} \in \mathbb{R}^n,$$

Function Ψ^* is the complex conjugate to Ψ, $\varkappa$ is a real parameter, $\hbar > 0$ is a small parameter. The operators $\hat{z}$ and $\hat{w}$ satisfy the following commutation relations

$$[\hat{z}_k, \hat{z}_j] = [\hat{w}_k, \hat{w}_j] = i\hbar J_{kj}, \tag{1.3}$$

$$[\hat{z}_k, \hat{w}_j] = 0, \qquad k,j = \overline{1,2n}, \tag{1.4}$$

where $J = \|J_{kj}\|_{2n\times 2n}$ is the standard symplectic matrix

$$J = \begin{pmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}_{2n\times 2n},$$

and $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ denotes the commutator of $\hat{A}$ and $\hat{B}$.

In this paper all functions of non-commutative operators are Weyl-ordered [41, 42]. The action of the operator $\hat{\mathcal{H}}$ in this case can be written as

$$\hat{\mathcal{H}}\Psi(\vec{x}, t, \hbar) = \frac{1}{(2\pi\hbar)^n} \int\limits_{\mathbb{R}^{2n}} d\vec{y}d\vec{p} \exp\Big(\frac{i}{\hbar}\ \langle \vec{x} - \vec{y}, \vec{p}\rangle\Big)\mathcal{H}\Big(\vec{p}, \frac{\vec{x}+\vec{y}}{2}\Big)\Psi(\vec{y}, t, \hbar), \tag{1.5}$$

where $\mathcal{H}(z) = \mathcal{H}(\vec{p}, \vec{x})$ is the Weyl symbol of the operator $\hat{\mathcal{H}}$, and $\langle \vec{x}, \vec{p}\rangle = \sum_{k=1}^{n} x_k p_k$.

Remark. In the particular case when the Weyl symbols of operators $\mathcal{H}(\hat{z})$ and $V(\hat{z}, \hat{w})$ in (1.2) have the form

$$\mathcal{H}(z) = \frac{\vec{p}^{\,2}}{2m} + U(\vec{x}), \quad V(z, w) = V(\vec{x}, \vec{y})$$

the equation (1.1) yields the equation of the self-consistent field in the form (0.8). This differential equation with integral nonlinearity plays a fundamental role in quantum theory and nonlinear optics [45, 46] and in the theory of the Bose-Einstein condensate [47]. In the latter the solution Ψ represents the wave function of the condensate, while the non-local potential $V(\vec{x}, \vec{y})$ describes the interaction of condensate's particles with external field.

In this paper we deal with asymptotic solutions of the equation (1.1) localized in the usual mathematical sense rather than in the sense of (0.6): namely, functions or formal series $\Psi(\vec{x}, t, \hbar)$ must belong to the Schwartz space with respect to the variables $\vec{x} \in \mathbb{R}^n$. We require the Weyl symbols $\mathcal{H}(z)$ and $V(z, w)$ of the operators $\hat{\mathcal{H}}$ and $V(\hat{z}, \hat{w})$ in (1.2) to belong to one of the T_+^m classes [3, p. 13]: they must be smooth functions of at most polynomial growth with all derivatives, such that the following conditions hold.

Assumption 1. *The functions $\mathcal{H}(z)$ and $V(z, w)$ are infinitely differentiable for all $z \in \mathbb{R}^{2n}$ and $w \in \mathbb{R}^{2n}$, and for any multi-indices α, $\mu \in \mathbb{Z}_+^{2n}$ there exist constants C_α, $C_{\alpha\mu}$ and $m \geqslant 0$ such that*

$$\Big|\frac{\partial^{|\alpha|}\mathcal{H}(z)}{\partial z^\alpha}\Big| \leqslant C_\alpha(1 + |z|)^m, \quad \Big|\frac{\partial^{|\alpha+\mu|}V(z, w)}{\partial z^\alpha \partial w^\mu}\Big| \leqslant C_{\alpha\mu}(1 + |z|)^m(1 + |w|)^m.$$

The notations here are as follows:

$$\begin{gathered} \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_{2n}), \quad \alpha_j \geqslant 0, \quad |\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_{2n}, \\ z^\alpha = z_1^{\alpha_1} z_2^{\alpha_2} \ldots z_{2n}^{\alpha_{2n}}, \qquad \frac{\partial^{|\alpha|}V(z)}{\partial z^\alpha} = \frac{\partial^{|\alpha|}V(z)}{\partial z_1^{\alpha_1}\partial z_2^{\alpha_2}\ldots\partial z_{2n}^{\alpha_{2n}}}. \end{gathered} \tag{1.6}$$

Note that for our method it is essential to have smooth symbols $\mathcal{H}(z)$ and $V(z, w)$. Asymptotics for Hartee-type equations with singularities are a subject of a number of publications, see e.g. [43] and references therein.

Now we introduce a vector space in which asymptotic solutions to the equation (1.1) will be sought.

2. Class of trajectory-coherent functions

We will construct asymptotic solutions of equation (1.1) with the following features: they have a form of generalized solitary waves and singularly depend of the small parameter $\hbar \to 0$.

Such a solution relies on a phase space trajectory $Z(t, \hbar) = (\vec{P}(t, \hbar), \vec{X}(t, \hbar))$ and is trajectory-coherent in the sense of (0.5), (0.4). We denote the class of trajectory-concentrated functions by $\mathcal{P}_\hbar^t(Z(t, \hbar))$ and define it more precisely as

$$\mathcal{P}_\hbar^t = \mathcal{P}_\hbar^t\big(Z(t, \hbar)\big) = \Big\{\Phi : \Phi(\vec{x}, t, \hbar) = \varphi\Big(\frac{\Delta\vec{x}}{\sqrt{\hbar}}, t, \hbar\Big) \exp\Big[\frac{i}{\hbar}(S(t, \hbar) + \langle \vec{P}(t, \hbar), \Delta\vec{x}\rangle)\Big]\Big\}, \tag{2.1}$$

where function $\varphi(\vec{\xi}, t, \hbar)$ belongs to the Schwartz space $\mathbb{S}$ with respect to variables $\vec{\xi} \in \mathbb{R}^n$, is a smooth function of t, and regularly depends on $\hbar$ as $\hbar \to 0$ (the term function is used throughout

in the sequel, although $\varphi(\vec{\xi},t,\hbar)$ may be in fact a formal series in powers of $\hbar^{1/2}$). Here $\Delta\vec{x}=\vec{x}-\vec{X}(t,\hbar)$. The real function $S(t,\hbar)$ and $2n$-vector-function $Z(t,\hbar)$ also regularly depend on $\hbar$ as $\hbar\to 0$. When an asymptotic solution of equation (1.1) is being constructed, these functions, as well as the amplitude $\varphi(\vec{\xi},t,\hbar)$ are to be determined. Short notation $\mathcal{P}_\hbar^t$ for $\mathcal{P}_\hbar^t(Z(t,\hbar))$ will be used when it does not lead to confusion, and $||\cdot||$ will denote the L_2-norm for functions from $\mathcal{P}_\hbar^t$. In the expression for the norm of a function from class $\mathcal{P}_\hbar^t$ the argument t may be omitted, and we write $\|\Phi(t)\|^2=\|\Phi\|^2$.

It will be shown in Section 3 that the functions $Z(t,\hbar)$ and $S(t,\hbar)$ are uniquely determined by the Ehrenfest system corresponding to the Hamiltonian of equation (1.1). In the linear case ($\varkappa=0$) the vector-function $Z(t,0)$ and the scalar function $S(t,0)$, defined by Hamiltonian function $\mathcal{H}(\vec{p},\vec{x})$, are the classical-mechanics phase space trajectory and the classical action respectively. As an example of amplitude, dynamical coherent states for quadratic Hamiltonians in the form of Gaussian function can be given:

$$\varphi(\vec{\xi},t)=\exp\Big[\frac{i}{2}\langle\vec{\xi},Q(t)\vec{\xi}\rangle\Big]f(t),$$

where $Q(t)$ is a complex symmetric matrix with positive imaginary part, and the time dependent factor $f(t)$ is given by

$$f(t)=\sqrt[4]{\mathrm{Im}\ Q(t)}\exp\Big[-\frac{i}{2}\int\limits_0^t \mathrm{Im}\ Q(\tau)\,d\tau\Big]$$

(see for details [16]).

Consider important properties of functions from class $\mathcal{P}_\hbar^t$. Their proofs are given in [16]. We briefly reproduce some of them in Appendix B.

1. Let Φ belong to the class $\mathcal{P}_\hbar^t(Z(t,\hbar))$. Introduce operator $\{\Delta\hat{z}\}^\alpha$ with Weyl symbol $(\Delta z)^\alpha=(\Delta z_1)^{\alpha_1}\cdot\ldots\cdot(\Delta z_{2n})^{\alpha_{2n}}$, and

$$\Delta z=z-Z(t,\hbar)=(\Delta\vec{p},\Delta\vec{x}),\qquad \Delta\vec{p}=\vec{p}-\vec{P}(t,\hbar),\qquad \Delta\vec{x}=\vec{x}-\vec{X}(t,\hbar).$$

Then the following asymptotic estimations for moments $\Delta_\alpha(t,\hbar)$ of order $|\alpha|$, $\alpha\in\mathbb{Z}_+^{2n}$ hold

$$\Delta_\alpha(t,\hbar)=\frac{\langle\Phi|\{\Delta\hat{z}\}^\alpha|\Phi\rangle}{\|\Phi\|^2}=O\big(\hbar^{|\alpha|/2}\big),\quad \hbar\to 0. \tag{2.2}$$

Denote by $\hat{O}(\hbar^\nu)$ an operator $\hat{F}$ such that for any function Φ, from the class $\mathcal{P}_\hbar^t(Z(t,\hbar))$, the asymptotic estimate holds

$$\frac{\|\hat{F}\Phi\|}{\|\Phi\|}=O(\hbar^\nu),\qquad \hbar\to 0.$$

2. The following asymptotic formula holds

$$\{\Delta\hat{z}\}^\alpha=\hat{O}(\hbar^{|\alpha|/2}),\quad \alpha\in\mathbb{Z}_+^{2n},\quad \hbar\to 0, \tag{2.3}$$

in particular

$$\{\Delta\hat{x}_k\}=\hat{O}(\hbar^{1/2}),\quad \{\Delta\hat{p}_j\}=\hat{O}(\hbar^{1/2}),\quad k,j=\overline{1,n}. \tag{2.4}$$

3. For functions $\Phi(\vec{x},t,\hbar)\in\mathcal{P}_\hbar^t(Z(t,\hbar))$ the following limits hold

$$\lim_{\hbar\to 0}\frac{1}{\|\Phi\|^2}|\Phi(\vec{x},t,\hbar)|^2=\delta(\vec{x}-\vec{X}(t,0)), \tag{2.5}$$

$$\lim_{\hbar\to 0}\frac{1}{\|\tilde{\Phi}\|^2}|\tilde{\Phi}(\vec{p},t,\hbar)|^2=\delta(\vec{p}-\vec{P}(t,0)), \tag{2.6}$$

where $\tilde{\Phi}(\vec{p},t,\hbar)=F_{\hbar,\vec{x}\to\vec{p}}\Phi(\vec{x},t,\hbar)$, $F_{\hbar,\vec{x}\to\vec{p}}$ is $\hbar^{-1}$-Fourier transform [3].

Denote by $\langle\hat{A}(t)\rangle_\Phi$ the mean value of a self-adjoint in $L_2(\mathbb{R}_x^n)$ operator $\hat{A}(t)$, $t\in\mathbb{R}^1$, calculated with respect to the function $\Phi(\vec{x},t,\hbar)\in\mathcal{P}_\hbar^t$. Then we have

4. For a function $\Phi(\vec{x},t,\hbar)\in\mathcal{P}^t_\hbar(Z(t,\hbar))$ and an operator $\hat{A}(t,\hbar)$ with Weyl symbol $A(z,t,\hbar)$ satisfying the first inequality in Assumption 1, the following equality holds

$$\lim_{\hbar\to0}\langle\hat{A}(t,\hbar)\rangle_\Phi=\lim_{\hbar\to0}\frac{1}{\|\Phi\|^2}\langle\Phi(\vec{x},t,\hbar)|\hat{A}(t,\hbar)|\Phi(\vec{x},t,\hbar)\rangle=A(Z(t,0),t,0). \tag{2.7}$$

The limiting nature of conditions (2.5), (2.6) and asymptotic character of estimations (2.2)–(2.4), holding in the class of trajectory-concentrated functions $\mathcal{P}^t_\hbar$ allows the construction of an approximate solution $\Psi_{\rm as}=\Psi_{\rm as}(\vec{x},t,\hbar)$ of the Hartree-type equation for any finite time interval $[0,T]$, in the following sense

$$\Big[-i\hbar\frac{\partial}{\partial t}+\hat{\mathcal{H}}+\varkappa\hat{V}(\Psi_{\rm as})\Big]\Psi_{\rm as}=O(\hbar^q), \tag{2.8}$$

$$\Psi_{\rm as}\in\mathcal{P}^t_\hbar(Z(t,\hbar),S(t,\hbar)),\quad t\in[0,T], \tag{2.9}$$

where $O(\hbar^q)$ denotes a function $g^{(q)}(\vec{x},t,\hbar)$ which represents the error for equation (1.1), and the error obeys the estimate

$$\max_{0\leqslant t\leqslant T}\|g^{(q)}(\vec{x},t,\hbar)\|=O(\hbar^q),\qquad\hbar\to0. \tag{2.10}$$

Following paper [16] and having in mind properties (2.5), (2.6), we call such a function $\Psi_{\rm as}(\vec{x},t,\hbar)$ a *semiclassically-concentrated solution* $(\mathrm{mod}\hbar^\alpha,\ \hbar\to0)$ for a Hartree-type equation (1.1).

The semiclassically concentrated $(\mathrm{mod}\hbar^\alpha)$ solution $\Psi^{(N)}(\vec{x},t,\hbar)$ of the Hartree-type equation is a formal asymptotic solution evolving from the initial state $\Psi_0(\vec{x},\hbar)$ chosen in the class of trajectory-concentrated functions $\mathcal{P}^0_\hbar(z_0,S_0)$. Here $z_0=(\vec{p}_0,\vec{x}_0)$ is an arbitrary point of the phase space $\mathbb{R}^{2n}_{px}$, and the constant $S_0=S(0,\hbar)$ can be set equal to zero without loss of generality We will denote the class of initial $(t=0)$ trajectory-concentrated functions by $\mathcal{P}^0_\hbar(z_0)$. Explicitly,

$$\mathcal{P}^0_\hbar\big(z_0\big)=\left\{\psi:\psi(\vec{x},\hbar)=\varphi_0\Big(\frac{\vec{x}-\vec{x}_0}{\sqrt{\hbar}},\hbar\Big)\exp\Big\{\frac{i}{\hbar}\langle\vec{p}_0,\vec{x}-\vec{x}_0\rangle\Big\},\quad\varphi_0(\vec{\xi},\hbar)\in\mathbb{S}(\mathbb{R}^n_\xi)\right\}, \tag{2.11}$$

Let us give two important examples of the amplitude function in the initial state (2.11).

First,

$$\varphi_0(\vec{\xi})=e^{-\langle\vec{\xi},A\vec{\xi}\rangle/2},$$

where the $n\times n$-matrix A is real symmetric and positive definite. In this case relation (2.11) describes the *Gaussian wave packet*.

Second,

$$\varphi_0(\vec{\xi})=e^{i\langle\vec{\xi},Q\vec{\xi}\rangle/2}H_\nu(\mathrm{Im}\,Q\vec{\xi}),$$

where the $n\times n$-matrix Q is complex symmetric and has positive definite imaginary part $\mathrm{Im}\,Q$, and $\nu=(\nu_1,\dots,\nu_n)$ is a multi-index of the multi-dimensional Hermite polynomial $H_\nu(\vec{\eta})$, $\vec{\eta}\in\mathbb{R}^n$ [48]. In this case $\psi\in\mathcal{P}^0_\hbar(z_0)$ (2.11) defines the *Fock state of a multi-dimensional oscillator*.

A construction of a semiclassically-concentrated solution $(\mathrm{mod}\hbar^\alpha)$, of the problem (1.1) with initial state from (2.11) is based on the solution of the Ehrenfest system, to which we turn our attention now.

3. The Ehrenfest system of equations

Let symbols $\mathcal{H}(z)$ $V(z,w)$ satisfy Assumption 1. Then operator $\mathcal{H}(\hat{z})$ (1.2) is self-adjoint with respect to inner product $\langle\Psi|\Phi\rangle$ in space $L_2(\mathbb{R}^n_x)$, and operator $V(\hat{z},\hat{w})$ (1.2) is self-adjoint for the inner product in space $L_2(\mathbb{R}^{2n}_{xy})$. Thus the norm of the exact solutions of (1.1) is preserved by time evolution: $\|\Psi(t)\|=\|\Psi_0\|$. The mean value $\langle\hat{A}\rangle=\langle\hat{A}\rangle_\Psi=\langle\Psi|\hat{A}|\Psi\rangle$ of an operator $\hat{A}(t)=A(\hat{z},t)$, calculated with respect to these solutions obeys

$$\frac{d}{dt}\langle\hat{A}(t)\rangle=\Big\langle\frac{\partial\hat{A}(t)}{\partial t}\Big\rangle+\frac{i}{\hbar}\langle[\mathcal{H}(\hat{z}),\hat{A}(t)]\rangle+\frac{i\varkappa}{\hbar}\Big\langle\int d\vec{y}\,\Psi^*(\vec{y},t,\hbar)[V(\hat{z},\hat{w}),\hat{A}(\hat{z},t)]\Psi(\vec{y},t,\hbar)\Big\rangle, \tag{3.1}$$

as an implication of the Heisenberg equation for evolution of operators. Equation (3.1) is called the *Ehrenfest equation for operator* $\hat{A}(t)$ *and function* $\Psi(\vec{x},t,\hbar)$. Our choice of this terminology is justified by analogy with the linear case $(\varkappa=0)$ in which equation (1.1) becomes the Schrödinger equation, while equation (3.1) is the Ehrenfest equation [4].

To derive the Ehrenfest system from the Ehrenfest equation (3.1) we take for Ψ a solution of the Hartree-type equation (1.1) in the class of trajectory-concentrated functions, and for $\hat{A}$ operators $\hat{z} = (\hat{\vec{p}}, \hat{\vec{x}})$ and $\{\Delta\hat{z}\}^\alpha$ with Weyl symbols $\{\Delta z\}^\alpha$, $\alpha \in \mathbb{Z}^{2n}_+$, where

$$\Delta z = z - Z(t,\hbar), \quad Z(t,\hbar) = \langle\Psi(t)|\hat{z}|\Psi(t)\rangle. \tag{3.2}$$

We represent operators $\mathcal{H}(\hat{z},t)$ and $V(\hat{z},\hat{w},t)$ in the series form

$$\mathcal{H}(\hat{z}) = \mathcal{H}(Z(t,\hbar)) + \sum_{|\mu|=1}^{\infty} \frac{1}{\mu!}\mathcal{H}_\mu(Z(t,\hbar))\{\Delta\hat{z}\}^\mu, \tag{3.3}$$

$$V(\hat{z},\hat{w}) = V(Z(t,\hbar),Z(t,\hbar)) + \sum_{|\nu|=1}^{\infty}\sum_{|\mu|=2}^{\infty} \frac{1}{\nu!\mu!}V_{\mu\nu}(Z(t,\hbar))\Delta_\mu\{\Delta\hat{z}\}^\nu,$$

$$\mathcal{H}_\mu(z,t) = \frac{\partial^{|\mu|}\mathcal{H}(z,t)}{\partial z^\mu}, \quad V_{\mu\nu}(z,t) = \frac{\partial^{|\mu+\nu|}V(z,w,t)}{\partial z^\mu \partial w^\nu}\Big|_{\omega=z}, \quad \mu,\nu \in \mathbb{Z}^{2n}_+,$$

where Δ_μ as defined in (2.2). Thus to derive the system we need to evaluate commutators $[\hat{z}_k, \{\Delta\hat{z}\}^\mu]$ and $[\{\Delta\hat{z}\}^\nu, \{\Delta\hat{z}\}^\mu]$ for $k = \overline{1,2n}$ and $|\mu| \geqslant 1$, $|\nu| \geqslant 1$. This has been done in the linear case ($\varkappa = 0$) [16, 22–24]) using the formula for composition of Weyl symbols $A(z)$ and $B(z)$ (see e.g. Appendix in [41]), defining the symbol $C(z)$ of the product of operators $\hat{C} = \hat{A}\,\hat{B}$

$$C(z) = A\Big(\overset{2}{z} + \frac{i\hbar}{2}J\frac{\overset{1}{\partial}}{\partial z}\Big)B(z) = B\Big(\overset{2}{z} - \frac{i\hbar}{2}J\frac{\overset{1}{\partial}}{\partial z}\Big)A(z). \tag{3.4}$$

Here the number over an operator refers to the order of its action onto the target function.

This way we obtain an infinite system of equations for $Z(t,\hbar), \Delta_\alpha(t,\hbar)$. Keeping only the moments up to order N, we obtain the following finite system of equations

$$\begin{aligned}
\dot{z} &= \sum_{|\mu|=0}^{N} \frac{1}{\mu!}J\Big(\mathcal{H}_{z\mu}(z)\Delta_\mu + \tilde{\varkappa}\sum_{|\nu|=0}^{N}\frac{1}{\nu!}V_{z\mu\nu}(z)\Delta_\mu\Delta_\nu\Big),\\
\dot{\Delta}_\alpha &= \sum_{|\mu+\gamma|=0}^{N}\Big(-i\hbar\Big)^{|\gamma|-1}\frac{[(-1)^{|\gamma_p|}-(-1)^{|\gamma_x|}]\alpha!\beta!\theta(\alpha-\gamma)\theta(\beta-\gamma)}{\gamma!(\alpha-\gamma)!(\beta-\gamma)!\mu!}\times\\
&\quad\times\Big(\mathcal{H}_\mu(z) + \tilde{\varkappa}\sum_{|\nu|=0}^{N}\frac{1}{\nu!}V_{\mu\nu}(z)\Delta_\nu\Big)\Delta_{\alpha-\gamma+J\beta-J\gamma} - \sum_{k=1}^{2n}\dot{Z}_k\alpha_k\Delta_{\alpha(k)}
\end{aligned} \tag{3.5}$$

with initial conditions

$$z\big|_{t=0} = z_0 = \langle\psi|\hat{z}|\psi\rangle, \qquad \Delta_\alpha\big|_{t=0} = \langle\psi|\{\hat{z}-z_0\}^\alpha|\psi\rangle, \qquad \alpha \in \mathbb{Z}^{2n}_+, \quad |\alpha| \leqslant N. \tag{3.6}$$

Here $\tilde{\varkappa} = \varkappa\|\psi(\vec{x},\hbar)\|^2$, and $\psi(\vec{x},\hbar)$ is the initial state from $\mathcal{P}^0_\hbar(z_0)$ (2.11),

$$\mathcal{H}_{z\mu}(z) = \frac{\partial^{|\mu|}\mathcal{H}_z(z)}{\partial z^\mu}, \quad V_{z\mu\nu}(z) = \frac{\partial^{|\mu+\nu|}V_z(z,w)}{\partial z^\mu\partial w^\nu}\Big|_{\omega=z}, \qquad \theta(\alpha-\beta) = \prod_{k=1}^{2n}\theta(\alpha_k-\beta_k), \tag{3.7}$$

$$\alpha = (\alpha_p,\alpha_x), \quad J\alpha = (\alpha_x,\alpha_p), \quad \alpha(k) = (\alpha_1-\delta_{k1},\dots,\alpha_{2n}-\delta_{k2n}).$$

As in the linear case ($\varkappa = 0$) (see [16]) the system (3.5) will be called *Ehrenfest system of order* N. Due to estimates (2.2) this system is equivalent in the class of trajectory-concentrated states to the Hartree-type equation (1.1) with precision $O(\hbar^{(N+1)/2})$.

Introduce notations

$$\begin{aligned}
&\mathfrak{H}(z,w) = \mathcal{H}(z) + \tilde{\varkappa}V(z,w), \quad \mathfrak{H}_z(z) = \mathfrak{H}_z(z,w)\Big|_{w=z} = \Big\|\frac{\partial\mathfrak{H}(z,w)}{\partial z_j}\Big|_{w=z}\Big\|_{1\times 2n},\\
&\mathfrak{H}_{zz}(z) = \mathfrak{H}_{zz}(z,w)\Big|_{w=z} = \Big\|\frac{\partial^2\mathfrak{H}(z,w)}{\partial z_j\partial z_k}\Big|_{w=z}\Big\|_{2n\times 2n}.
\end{aligned} \tag{3.8}$$

Then for $N = 0$ the Ehrenfest system (3.5) has the form

$$\dot{z} = J\mathfrak{H}_z(z), \tag{3.9}$$

and for $N = 2$ we obtain

$$\begin{cases} \dot{z} = J\partial_z \Big[1 + \frac{1}{2}\langle \partial_z, \Delta_2 \partial_z\rangle + \frac{1}{2}\langle \partial_w, \Delta_2 \partial_w\rangle\Big] \mathfrak{H}(z,w)\Big|_{w=z}, \\ \dot{\Delta}_2 = J\mathfrak{H}_{zz}(z)\Delta_2 - \Delta_2 \mathfrak{H}_{zz}(z) J, \quad \Delta_2^{\intercal} = \Delta_2, \end{cases} \tag{3.10}$$

where Δ_2 is a symmetric $(2n \times 2n)$-matrix of the second moments ($\Delta_2 = \|\Delta_{ji}\|_{2n\times 2n}$)

$$\Delta_2(t) = \begin{pmatrix} \sigma_{pp}(t) & \sigma_{px}(t) \\ \sigma_{xp}(t) & \sigma_{xx}(t) \end{pmatrix}, \tag{3.11}$$

with $(n \times n)$-blocks

$$\sigma_{pp}(t) = \|\sigma_{p_k p_l}(t)\|_{n\times n} = \|\langle \Delta\hat{p}_k \Delta\hat{p}_l\rangle)\|_{n\times n}, \quad \sigma_{xx}(t) = \|\sigma_{x_k x_l}(t)\|_{n\times n} = \|\langle \Delta x_k \Delta x_l\rangle\|_{n\times n},$$
$$\sigma_{xp}(t) = \|\sigma_{x_k p_l}(t)\|_{n\times n} = \Big\|\frac{1}{2}\langle \Delta x_k \Delta\hat{p}_l + \Delta\hat{p}_l \Delta x_k\rangle\Big\|_{n\times n};$$

System (3.10) can be written in an equivalent form introducing matrix $A(t)$ via relation

$$\Delta_2(t) = A(t)\Delta_2(0)A^{+}(t).$$

Then the system becomes

$$\begin{cases} \dot{z} = J\partial_z \Big[1 + \frac{1}{2}\langle \partial_z, A\Delta_2^0 A^{+} \partial_z\rangle + \frac{1}{2}\langle \partial_w, A\Delta_2^0 A^{+} \partial_w\rangle\Big] \mathfrak{H}(z,w)\Big|_{w=z}, \\ \dot{A} = J\mathfrak{H}_{zz}(z)A, \qquad A(0) = \mathbb{I}. \end{cases} \tag{3.12}$$

Note that the initial state function can be excluded from the initial conditions (3.6) for the system (3.10) if they satisfy an infinite system of inequalities [4] (generalized Heisenberg uncertainty conditions) and for $t = 0$ satisfy estimations (2.2). Obviously, all Heisenberg inequalities are consistent with equations (3.5).

The uncertainty relation corresponding to the Ehrenfest system (3.10) can be rewritten as the condition that matrix $\Delta_2(t) + \frac{i\hbar}{2}J$ is positive definite [50] (see also [16, 51]).

The fact that equation (3.5) is a finite system of ordinary differential equations for functions z, Δ_α equivalent to problem (1.1) with precision $O(\hbar^{(N+1)/2})$, suggests that there is a mechanical system with finite degrees of freedom described by (3.5), and thus an approximate semiclassical model of a Hartree-type equation allows an exact interpretation in frame of classical mechanics. The number of degrees of freedom of such a mechanical system grows with precision N. A study of such classical systems with quantum origin by methods of classical mechanics constitutes a separate interesting direction of research [27, 28].

4. The Ehrenfest system: the small dispersions approximation

Denote by $\hat{\mathfrak{g}}$ operators

$$\hat{\mathfrak{g}} = \left(\hat{z}_j, \hat{\Delta}_2^{kl} = \frac{1}{2}(\Delta\hat{z}_k \Delta\hat{z}_l + \Delta\hat{z}_l \Delta\hat{z}_k); \quad j,k,l = \overline{1,2n}, k \leqslant l\right). \tag{4.1}$$

Their mean values in state $\Psi(\vec{x},t)$ with initial condition $\Psi(\vec{x},t)\Big|_{t=0} = \psi(\vec{x})$, are denoted by

$$\mathfrak{g}_\psi(t,\hbar) = \langle \Psi(\vec{x},t)|\hat{\mathfrak{g}}|\Psi(\vec{x},t)\rangle = \left(Z(t,\hbar,\mathfrak{g}_\psi^0), \Delta_2(t,\hbar,\mathfrak{g}_\psi^0)\right). \tag{4.2}$$

The mean values $\mathfrak{g}_\psi(t,\hbar)$ obey Ehrenfest system (3.10) with initial condition $\mathfrak{g}_\psi(0,\hbar) = \mathfrak{g}_\psi^0 = \langle\psi|\hat{\mathfrak{g}}|\psi\rangle$. When it does not lead to confusion the explicit dependence of the initial function will be omitted in the notations.

[4] For $|\alpha+\beta| \leqslant 4$ the system of inequalities is well known (see e.g. [51], and the bibliography there).

Estimations (2.2) suggest that the Ehrenfest system can be solved approximatly with respect to a small parameter $\hbar$ using the expansions

$$\mathfrak{g}(t,\hbar) = \mathfrak{g}^{(0)}(t,\hbar) + \hbar\mathfrak{g}^{(1)}(t,\hbar) + \dots, \tag{4.3}$$

or

$$\begin{aligned} Z(t) &= Z^{(0)}(t) + \hbar Z^{(1)}(t) + \dots, \\ \Delta_2(t) &= \Delta_2^{(0)}(t,\hbar) + \hbar\Delta_2^{(1)}(t,\hbar) + \dots. \end{aligned} \tag{4.4}$$

Here $\mathfrak{g}^{(0)}(t,\hbar) = \left(Z^{(0)}(t), \Delta_2^{(0)}(t,\hbar)\right)$ is the principal term of the solution of system (3.10). Substituting (4.3) into system (3.10) we obtain equations for $z^{(0)} = Z^{(0)}$, $z^{(1)} = Z^{(1)}$, and $\Delta_2^{(0)}$ with precision $O(\hbar^{3/2})$

$$\left\{ \begin{array}{l} \dot{z}^{(0)} = J\mathfrak{H}_z(z^{(0)}), \\ \dot{z}^{(1)} = J\mathfrak{H}_{zz}(z^{(0)})z^{(1)} + F(z^{(0)}, \Delta_2^{(0)}), \\ \dot{\Delta}_2^{(0)} = J\mathfrak{H}_{zz}(z^{(0)})\Delta_2^{(0)} - \Delta_2^{(0)}\mathfrak{H}_{zz}(z^{(0)})J. \end{array} \right. \tag{4.5}$$

Here

$$F(z,\Delta_2) = \frac{1}{2\hbar} J\partial_z \operatorname{Sp}\left\{ \left[\mathfrak{H}_{zz}(z,w) + \tilde{\varkappa} V_{ww}(z,w) \right] \Delta_2 \right\}\Big|_{w=z}. \tag{4.6}$$

The first equation of system (4.5) coincides with (3.9) and is similar to the classical-mechanical Hamilton system in the linear case, however, in the nonlinear case ($\tilde{\varkappa} \neq 0$) the system is not Hamiltonian.

Consider the following auxiliary system of equations which can be referred as the *pseudo-system-in-variations* for the solution $Z^{(0)}(t)$

$$\dot{a}_k = J\mathfrak{H}_{zz}(Z^{(0)}(t))a_k \quad k = \overline{1,n}, \tag{4.7}$$

with normalization condition

$$\{a_k(t), a_l(t)\} = \{a_k^*(t), a_l^*(t)\} = 0, \quad \{a_k^*(t), a_l(t)\} = -2i\delta_{kl}, \tag{4.8}$$

where $\{v,u\}$ is a skew symmetric inner product in $\mathbb{R}^{2n}$

$$\begin{gathered} \{v,u\} = \langle v, J^\intercal u\rangle = \vec{W}_a^\intercal \vec{Y}_b - \vec{Y}_a^\intercal \vec{W}_b, \\ v = \begin{pmatrix} \vec{W}_a \\ \vec{Y}_a \end{pmatrix}, \quad u = \begin{pmatrix} \vec{W}_b \\ \vec{Y}_b \end{pmatrix}. \end{gathered} \tag{4.9}$$

If a solution $z^{(0)} = Z^{(0)}(t)$ as well as a complete set of solutions $a_k(t)$ of the pseudo-system-in-variation are known then the general solution of the two last equations in (4.5) has the form

$$Z^{(1)}(t) = \sum_{k=1}^{n} \left[b_k(t)a_k(t) + b_k^*(t)a_k^*(t) \right], \tag{4.10}$$

$$\Delta_2^{(0)}(t) = A(t)\mathcal{D}A^t(t), \tag{4.11}$$

where scalar functions $b_k(t)$ and the $2n \times 2n$-matrix $A(t)$ are as follows

$$b_k(t) = -\frac{1}{2i}\int_0^t \{a_k^*(t), \tilde{F}(t)\}dt + b_k, \quad \tilde{F}(t) = F(Z^{(0)}(t), \Delta_2^{(0)}(t)), \tag{4.12}$$

$$A(t) = \Big(a_1(t), a_2(t), \dots, a_n(t), a_1^*(t), a_2^*(t), \dots, a_n^*(t)\Big). \tag{4.13}$$

Here b_k are constants of integration, $\mathcal{D}$ is an arbitrary $2n\times 2n$ constant matrix and $F(Z^{(0)}(t), \Delta_2^{(0)}(t))$ is defined in (4.6). Thus in this approximation the total solution is determined by solutions of the modified classical system (3.9) and pseudo-system-in-variations (4.7).

5. Energy spectrum and the Ehrenfest system for quantum means.

Consider the problem of defining the energy spectrum for a Hartree-type Hamiltonian $\hat{\mathcal{H}}_\varkappa$ from the dynamical Ehrenfest system for quantum means. Denote by $S[\mathfrak{g}_\psi(t,\hbar)]$ the generalized action [36, 37] along the trajectory $\mathfrak{g}_\psi(t,\hbar)$ (4.2) of the Ehrenfest system (3.10)

$$S\Big[\mathfrak{g}_\psi(t,\hbar)\Big] = \int\limits_0^t dt\Big[\Big\langle \vec{P}(t,\mathfrak{g}^0_\psi), \dot{\vec{X}}(t,\mathfrak{g}^0_\psi)\Big\rangle - \mathfrak{H}\Big(z,w\Big) - \frac{\tilde{\varkappa}}{2}\mathrm{Sp}\Big(V_{ww}(z,w)\Delta_2(t,\mathfrak{g}^0_\psi)\Big)\Big]\Big|_{w=z=Z(t,\mathfrak{g}^0_\psi)} -$$
$$-\hbar\Big\langle P^{(0)}(t,\mathfrak{g}^0_\psi), X^{(1)}(t,\mathfrak{g}^0_\psi)\Big\rangle + \hbar\langle p_0, X^{(1)}_0\rangle. \tag{5.1}$$

Substituting (4.4) in (5.1) we get

$$S\Big[\mathfrak{g}_\psi(t,\hbar)\Big] = \int\limits_0^t dt\Big[\Big\langle \vec{P}^{(0)}(t,\mathfrak{g}^0_\psi), \dot{\vec{X}}^{(0)}(t,\mathfrak{g}^0_\psi)\Big\rangle - \mathfrak{H}\Big(z,w\Big) -$$
$$-\hbar\tilde{\varkappa}\langle V_w(z,w), Z^{(1)}(t,\mathfrak{g}^0_\psi)\rangle - \frac{\tilde{\varkappa}}{2}\mathrm{Sp}\Big(V_{ww}(z,w)\Delta^{(0)}_2(t,\mathfrak{g}^0_\psi)\Big)\Big]\Big|_{w=z=Z^{(0)}(t,\mathfrak{g}^0_\psi)} + O(\hbar^{3/2}). \tag{5.2}$$

The connection between the energy spectrum and the time-dependent solution $\mathfrak{g}_\psi(t,\hbar)$ is established as follows

Statement 5.1. *Let the Hartree-type stationary equation*

$$\widehat{\mathcal{H}}_\varkappa(\varphi_\nu)\varphi_\nu = E_\nu\varphi_\nu, \qquad \nu \in \mathbb{Z}^n_+ \tag{5.3}$$

have pure discrete non-degenerate spectrum, and functions φ_ν form a basis in $\mathcal{P}^0_\hbar(z_0)$ (2.11). Let a solution $\mathfrak{g}(t,\hbar)$ of system (3.10) exist in the class of quasi-periodic functions [49]:

$$\mathfrak{g}(t,\hbar) = \sum_{|\nu+\nu'|=0}^{\infty} \mathfrak{g}_{\nu\nu'}(\hbar)e^{i\omega_{\nu\nu'}t}, \tag{5.4}$$

and satisfy the generalized Heisenberg inequalities. Here $\mathfrak{g}_{\nu\nu'}(\hbar)$ are generalized Fourier coefficients for function $\mathfrak{g}(t,\hbar)$. Then the energy levels E_ν and the frequencies $\omega_{\nu\nu'}$ are connected by the following relation (mod $\hbar^{3/2}$)

$$\hbar\omega_{\nu\nu'} = E_\nu - E_{\nu'} + \frac{1}{t}S[\mathfrak{g}_{\varphi_\nu}(t,\hbar)] - \frac{1}{t}S[\mathfrak{g}_{\varphi_{\nu'}}(t,\hbar)], \qquad \nu\nu' \in \mathbb{Z}^n_+. \tag{5.5}$$

Proof. At the initial moment of time function $\mathfrak{g}(t,\hbar)$ satisfies the generalized Heisenberg inequalities. Thus there exists a function $\psi \in \mathcal{P}^0_\hbar(z_0)$ such that with the accuracy $O(\hbar^{3/2})$, $\mathfrak{g}(0,\hbar) = \mathfrak{g}_\psi(0,\hbar) = \langle\psi|\hat{\mathfrak{g}}|\psi\rangle$ (see [16]).

Since vectors φ_ν form a complete set and belong to $\mathcal{P}^0_\hbar(z_0)$, every semiclassically-concentrated solution of (1.1) with the same Hamiltonian as in (5.3), and initial state $\psi \in \mathcal{P}^0_\hbar(z_0)$, can be represented in the form (see Appendix A):

$$\Psi(\vec{x},t) = \exp\Big(\frac{i}{\hbar}S[\mathfrak{g}_\psi(t,\hbar)]\Big)\sum_{|\nu|=0}^{\infty} C_\nu \exp\Big(-\frac{i}{\hbar}E_\nu t - \frac{i}{\hbar}S[\mathfrak{g}_{\varphi_\nu}(t,\hbar)]\Big)\varphi_\nu(\vec{x}) + O(\hbar^{3/2}). \tag{5.6}$$

Using function $\Psi(\vec{x},t)$ in this form for evaluation of the mean value of operators $\hat{\mathfrak{g}}$ (4.1) and comparing with (5.4) we get (5.5), which completes the proof.

If the ground level of energy E_0 as well as the complete set of frequencies $\omega_{\nu\nu'}$ are given, then the problem of reconstruction of the entire spectrum E_ν is a well known problem in spectroscopy.

The invariant manifolds of classical Hamiltonian systems are known to be important for classification of spectral series in the linear theory ($\varkappa = 0$) [10].

We are able to solve the problem in the semiclassical approximation using invariant manifolds $\mathfrak{g}^{(0)}(t)$ of system (4.5) for classification of the spectral series.

In the simplest case when the invariant set consists of a single rest point $z^{(0)} = Z^{(0)}(t) = \text{const}$ it follows from (4.5) that

$$\mathfrak{H}_z(z^{(0)}) = \partial_z \Big[\mathcal{H}(z) + \tilde{\varkappa} V(z,w) \Big] \Big|_{w=z=z^{(0)}} = 0. \tag{5.7}$$

Identify the rest point $Z^{(0)}$ with point z_0 which defines class $\mathcal{P}^0_\hbar(z_0)$ (2.11). In other words we take initial states localized at the rest point $z_0 = Z^{(0)}$.

We will proceed under the following assumption.

Assumption 2. *Let the symplectic $(2n \times 2n)$-matrix $J\mathfrak{H}_{zz}(z_0)$ evaluated at the rest point z_0 have n distinct pure imaginary eigenvalues $i\Omega_k$, $\Omega_k > 0$, $k = \overline{1,n}$ (and n eigenvalues complex conjugate to them, $-i\Omega_k$, $k = \overline{1,n}$).*

In the linear theory, Assumption 2 implies stability of the rest point in the linear approximation [9].

Note that under Assumption 2, solutions of the pseudo-system-in-variation (4.7) have the form

$$a_k(t) = \exp(i\Omega_k t) f_k, \quad k = \overline{1,n}, \tag{5.8}$$

where f_k is the eigenvector of the pseudo-matrix-in-variations, evaluated at the rest point

$$J\mathfrak{H}_{zz}(z_0) f_k = i\Omega_k f_k, \qquad \Omega_k \neq \Omega_j, \quad j,k = \overline{1,n}. \tag{5.9}$$

The eigenvectors f_k, $k = \overline{1,n}$ are normalized, without loss of generality, by condition (4.8).

Statement 5.2. *Under Assumption 2, the energy spectrum of the Hartree-type operator* (5.3) *can be found as*

$$E_\nu = \mathfrak{H}(z_0,z_0) + \hbar \sum_{k=1}^n \widetilde{\Omega}_k \left(\nu_k + \frac{1}{2} \right) + O(\hbar^{3/2}), \tag{5.10}$$

where multi-index $\nu = (\nu_1, \dots, \nu_n)$ has all non-negative components, $\mathfrak{H}(z,w)$ is defined in (3.8) *and*

$$\begin{aligned} \widetilde{\Omega}_k = \Omega_k + \frac{\tilde{\varkappa}}{2} \langle f_k^*, V_{ww}(z_0,z_0) f_k \rangle + \\ + \operatorname{Re} \sum_{j=1}^n \frac{\tilde{\varkappa}}{2\Omega_j} \langle V_w(z_0,z_0), f_k \rangle \langle f_k^*, \partial_z \rangle \langle f_j^*, [\mathfrak{H}_{zz}(z,w) + \tilde{\varkappa} V_{ww}(z,w)] f_j \rangle \Big|_{z=w=z_0}. \end{aligned} \tag{5.11}$$

For $\nu = 0$ our result (5.10) coincides with results obtained in [52] with precision $O(\hbar^{3/2})$.

To prove Statement 5.2 we need several Lemmas.

Lemma 5.1. *Under Assumption 2, the spectrum of Hartree-type operator* (5.3) *is equidistant* ($\operatorname{mod} \hbar^{3/2}$) *and can be found as*

$$E_\nu = E_0 + \hbar \sum_{k=1}^n \widetilde{\Omega}_k \nu_k, \tag{5.12}$$

where $E_0 = \text{const}$ is the ground energy level and $\widetilde{\Omega}_k$ are defined in (5.11).

Proof. As the first step, we establish the linear relation between Ω_k, $k = \overline{1,n}$ and $\omega_{\nu\nu'}$ in the Statement 5.1. Using (5.8), formulas (4.10) and (4.11) with (4.6), (4.12), (4.13) become

$$\begin{aligned} Z^{(1)}(t) &= \sum_{k=1}^n \operatorname{Re} \left[\{ f_k^*, \mathfrak{F}_k(t) \} f_k + b_k e^{i\Omega_k t} f_k \right], \qquad b_k = \text{const}, \\ \Delta_2^{(0)}(t) &= \sum_{j,l=1}^n \frac{1}{2} \left(f_j f_l^+ + f_j^* f_l^\intercal \right) \mathcal{D}_{jl} e^{i(\Omega_j - \Omega_l)t}, \quad f_l^+ = (f_l^*)^\intercal, \quad \mathcal{D}_{jl} = \text{const}. \end{aligned} \tag{5.13}$$

Here the $2n$-vector $\mathfrak{F}_k(t)$ is defined by the relation

$$\mathfrak{F}_k(t) = \frac{1}{2\hbar} J \partial_z \operatorname{Sp} \left\{ \Big[\mathfrak{H}_{zz}(z,w) + \tilde{\varkappa} V_{ww}(z,w) \Big] \mathcal{F}_k(t) \right\} \Big|_{w=z=z_0}, \tag{5.14}$$

where the $(2n \times 2n)$-matrix $\mathcal{F}_k(t)$ has the following structure

$$\mathcal{F}_k(t) = \sum_{j,l=1}^{n} \frac{1}{2(\Omega_k + \Omega_j - \Omega_l)} \left(f_j f_l^+ + f_j^* f_l^\intercal \right) \mathcal{D}_{jl} e^{i(\Omega_j - \Omega_l)t}. \tag{5.15}$$

Using the estimate (2.2), solution of the Ehrenfest system (3.5) can be written in the form

$$\mathfrak{g}(t,\hbar) = \left(z_0 + \hbar Z^{(1)}(t), \Delta_2^{(0)}(t) \right) + O(\hbar^{3/2}). \tag{5.16}$$

Introduce vectors

$$\vec{\mu} = (\mu_1, \ldots, \mu_n), \quad \vec{\nu} = (\nu_1, \ldots, \nu_n), \quad \vec{\Omega} = (\Omega_1, \ldots, \Omega_n), \tag{5.17}$$

and let $|\vec{\mu}|$ denote the sum of the absolute values of vector's components. Substitute (5.13) into (5.16) and rewrite it as

$$\mathfrak{g}(t,\hbar) = \sum_{|\vec{\mu}| \leqslant 2} \mathfrak{g}_\mu(\hbar) e^{i\langle \vec{\mu}, \vec{\Omega} \rangle t} + O(\hbar^{3/2}). \tag{5.18}$$

The right hand side in (5.18) is an almost periodic function with n frequencies $\Omega_1, \ldots \Omega_n$. The exponents in (5.18) are linear combinations of the frequencies Ω_k, $k = \overline{1,n}$ with integer coefficients μ_k, and thus linearly depend on the multi-index $\mu \in \mathbb{Z}_+^n$. Consequently, frequencies $\omega_{\nu\nu'}$ (5.4), must be linear functions of ν and ν'. Taking into account that by interchanging ν and ν' frequencies $\omega_{\nu\nu'}$ (5.5) change sign, and by preceding arguments, we get

$$\omega_{\nu\nu'} = \langle \vec{\nu} - \vec{\nu}', \vec{\Omega} \rangle = \langle \vec{\mu}, \vec{\Omega} \rangle, \quad |\vec{\mu}| \leqslant 2. \tag{5.19}$$

The step 2 of our proof consists in recalculation of the right hand side of the formula (5.5).

Energy level E_ν with precision $O(\hbar^{3/2})$ can be found from the mean value of $\hat{\mathcal{H}}_\varkappa$ in the stationary state $\varphi_\nu \in \mathcal{P}_\hbar^0(z_0)$ as follows

$$\begin{aligned} E_\nu = \langle \varphi_\nu | \hat{\mathcal{H}}_\varkappa(\varphi_\nu) | \varphi_\nu \rangle = \mathfrak{H}(z_0, z_0) + \hbar\tilde{\varkappa} \langle V_w(z_0, z_0), Z_\nu^{(1)} \rangle + \\ + \frac{1}{2} \operatorname{Sp} \left\{ \Big[\mathfrak{H}_{zz}(z_0) + \tilde{\varkappa} V_{ww}(z_0, z_0) \Big] \Delta_2^\nu \right\} + O(\hbar^{3/2}). \end{aligned} \tag{5.20}$$

Here the equality (5.7) was used.

Note that for the stationary state φ_ν we have for coefficients in (5.13) $b_k^\nu = 0$, $\mathcal{D}_{jl}^\nu = \mathcal{D}_l^{(\nu)} \delta_{jl}$ since the functions are time-independent

$$Z_\nu^{(1)} = \sum_{k=1}^{n} \operatorname{Re}[\{f_k^*, \mathfrak{F}_k^\nu\} f_k], \qquad \Delta_2^\nu = \sum_{l=1}^{n} \frac{1}{2} \left(f_l f_l^+ + f_l^* f_l^\intercal \right) \mathcal{D}_l^{(\nu)}. \tag{5.21}$$

Here vector $\mathfrak{F}_k^\nu$ is defined by (5.14) with

$$\mathcal{F}_k(t) = \mathcal{F}_k^\nu = \sum_{j=1}^{n} \frac{1}{2\Omega_k} \mathcal{D}_j^{(\nu)} \left(f_j f_j^+ + f_j^* f_j^\intercal \right). \tag{5.22}$$

Substituting formulas (5.21) into (5.20) we get after some calculations using (5.9)

$$E_\nu = \mathfrak{H}(z_0, z_0) + \hbar\tilde{\varkappa} \langle V_w(z_0, z_0), Z_1^{(\nu)} \rangle + \sum_{k=1}^{n} \Big[\Omega_k + \frac{\tilde{\varkappa}}{2} \langle f_k^*, V_{ww}(z_0, z_0) f_k \rangle \Big] \mathcal{D}_k^{(\nu)} + O(\hbar^{3/2}) \tag{5.23}$$

Similarly, from (5.2) we find

$$\frac{1}{t} S[\mathfrak{g}_{\varphi_\nu}] = -\mathfrak{H}(z_0, z_0) - \hbar\tilde{\varkappa} \langle V_w(z_0, z_0), Z_1^{(\nu)} \rangle - \tilde{\varkappa} \sum_{k=1}^{n} \langle f_k^*, V_{ww}(z_0, z_0) f_k \rangle \mathcal{D}_k^{(\nu)}, \tag{5.24}$$

Now substitute (5.23),(5.24) in (5.5) to find that

$$\hbar\omega_{\nu\nu'} = \sum_{j=1}^{n} \Omega_j (D_j^{(\nu)} - D_j^{(\nu')}).$$

From this equation along with (5.19) we can find $D_j^{(\nu)}$ in terms of $D_j^{(0)}$ as follows

$$\mathcal{D}_j^{(\nu)} = \mathcal{D}_j^{(0)} + \hbar\nu_j, \quad j = \overline{1,n}. \tag{5.25}$$

Constants $\mathcal{D}_j^{(0)}$ will be defined later.

To illustrate how the equation (5.25) was obtained we temporarily consider case $n = 2$, without loss of generality. Then condition $|\vec{\mu}| \leqslant 2$ in (5.19) reduces our consideration effectively to the three cases.

Case 1. If $\mu_1 = 1$, $\mu_2 = 0$ then $\omega_{\nu\nu'} = \Omega_1$ and $\nu_1 - \nu_1' = 1$, $\nu_2 - \nu_2' = 0$. Consequently,

$$\hbar\Omega_1 = \Omega_1(D_1^{(\nu_1,\nu_2)} - D_1^{(\nu_1-1,\nu_2)}) + \Omega_2(D_2^{(\nu_1,\nu_2)} - D_2^{(\nu_1-1,\nu_2)}),$$

and thus

$$D_1^{(\nu_1,\nu_2)} = D_1^{(\nu_1-1,\nu_2)} + \hbar, \quad D_2^{(\nu_1,\nu_2)} = D_2^{(\nu_1-1,\nu_2)}.$$

Case 2. If $\mu_1 = 0$, $\mu_2 = 1$ then $\omega_{\nu\nu'} = \Omega_2$ and $\nu_1 - \nu_1' = 0$, $\nu_2 - \nu_2' = 1$. Consequently,

$$\hbar\Omega_2 = \Omega_1(D_1^{(\nu_1,\nu_2)} - D_1^{(\nu_1,\nu_2-1)}) + \Omega_2(D_2^{(\nu_1,\nu_2)} - D_2^{(\nu_1,\nu_2-1)}),$$

and thus

$$D_1^{(\nu_1,\nu_2)} = D_1^{(\nu_1,\nu_2-1)}, \quad D_2^{(\nu_1,\nu_2)} = D_2^{(\nu_1,\nu_2-1)} + \hbar.$$

Case 3. If $\mu_1 = 1$, $\mu_2 = 1$ then $\omega_{\nu\nu'} = \Omega_1 + \Omega_2$ and $\nu_1 - \nu_1' = 1$, $\nu_2 - \nu_2' = 1$. Consequently,

$$\hbar(\Omega_1 + \Omega_2) = \Omega_1(D_1^{(\nu_1,\nu_2)} - D_1^{(\nu_1-1,\nu_2-1)}) + \Omega_2(D_2^{(\nu_1,\nu_2)} - D_2^{(\nu_1-1,\nu_2-1)}),$$

and thus

$$D_1^{(\nu_1,\nu_2)} = D_1^{(\nu_1-1,\nu_2-1)} + \hbar, \quad D_2^{(\nu_1,\nu_2)} = D_2^{(\nu_1-1,\nu_2-1)} + \hbar.$$

Note that the third case result can be decomposed into the first two. It is apparent that similar derivations are possible in any dimension $n \geqslant 2$, and that equation (5.25) holds.

As the third step of the proof, we finally obtain the statement of Lemma 5.1. Using (5.21) for $Z_\nu^{(1)}$ with (5.22) for $\mathfrak{F}_k^\nu$, from (4.6) and (5.13), we find

$$\begin{aligned}\langle V_w(z_0,z_0), Z_1^{(\nu)}\rangle = \operatorname{Re}\sum_{k=1}^{n}\sum_{j=1}^{n}\frac{1}{2\Omega_j}\langle V_w(z,w), f_k\rangle\times \\ \times\langle f_k^*, \partial_z\rangle\Big\langle f_j^*, \Big[\mathfrak{H}_{zz}(z,w) + \tilde{\varkappa}V_{ww}(z,w)\Big]\Big|_{z=w=z_0} f_j\Big\rangle\mathcal{D}_j^{(\nu)}.\end{aligned} \tag{5.26}$$

From (5.23), using (5.25) and (5.26) we get

$$E_\nu = \mathfrak{H}(z_0,z_0) + \sum_{j=1}^{n}\widetilde{\Omega}_j\Big[\mathcal{D}_j^{(0)} + \hbar\nu_j\Big], \tag{5.27}$$

where $\widetilde{\Omega}_j$ is given by (5.11). Finally, denote by

$$E_0 = \mathfrak{H}(z_0,z_0) + \sum_{j=1}^{n}\widetilde{\Omega}_j\mathcal{D}_j^{(0)} \tag{5.28}$$

to obtain (5.12). Thus the lemma is proved.

Lemma 5.2. *Under Assumption 2, the ground energy level for the Hartree-type operator* (5.3) *is given (*mod $\hbar^{3/2}$*) by*

$$E_0 = \mathfrak{H}(z_0,z_0) + \frac{\hbar}{2}\sum_{j=1}^{n}\widetilde{\Omega}_j. \tag{5.29}$$

Proof. The ground energy level E_0 is given by (5.28), which follows from (5.27) for $\nu = 0$. Constants $\mathcal{D}_k^{(0)}$ will be chosen in order to minimize the uncertainty condition and obey the quantization condition (5.5). This idea is supported by physical models including the harmonic oscillator and the Coulomb potential [53, 54] (see [51] and references there).

As we have mentioned above, matrix $\Delta_2(t) + \frac{i\hbar}{2}J$ is positive definite. Thus for any vector v we have

$$v^+\left[\Delta_2(t) + \frac{i\hbar}{2}J\right]v \geqslant 0,$$

where equality corresponds to minimization of the uncertainty relation.

Take $v = Jf_j, j = \overline{1,n}$. Then using (5.21) with $\nu = 0$ and orthogonal condition (4.8) (which is valid for vectors f_k, as well as for $a_k(t)$) we have

$$\mathcal{D}_j^{(0)} \geqslant \frac{\hbar}{2}.$$

So, choosing

$$\mathcal{D}_j^{(0)} = \frac{\hbar}{2}, \tag{5.30}$$

we minimize the uncertainty relation, and obtain (5.29).

Then formula (5.10) directly follows from (5.12) and (5.29). Thus statement 5.2 is proved.

6. Spectrum for the oscillator with nonlinear Gaussian potential

6.1. Spectrum for the oscillator in constant magnetic field and nonlinear Gaussian potential.

In this section we illustrate the method described above with an example of a Hartree-type equation (1.1) whose linear part corresponds to an oscillator in a constant magnetic field, while the nonlinear part is described via Gaussian potential. The linear part $\hat{\mathcal{H}}$ has the form

$$\hat{\mathcal{H}} = \frac{1}{2m}(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\vec{x}))^2 + \frac{k}{2}\vec{x}^2. \tag{6.1}$$

The external field in the operator (6.1) is a superposition of a constant magnetic field $\vec{H} = (0, 0, H)$ with vector potential $\vec{A} = \frac{1}{2}\vec{H} \times \vec{x}$ and an oscillatory field with scalar potential $\frac{k}{2}\vec{x}^2$. The non-local operator $\hat{V}(\Psi)$ in (1.2) has the form

$$\hat{V}(\Psi) = \int_{\mathbb{R}^3} V(\vec{x}, \vec{y})|\Psi(\vec{y}, t)|^2 d\vec{y}, \qquad V(\vec{x}, \vec{y}) = V_0 \exp\left[-\frac{(\vec{x} - \vec{y})^2}{2\gamma^2}\right]. \tag{6.2}$$

Here H, V_0, k, γ, e, c are real parameters of the model.

We will be using notations ω_H, ω_0, and ω_{nl} for the cyclotron frequency, oscillator frequency, and nonlinear frequency respectively

$$\omega_H = \frac{eH}{mc}, \qquad \omega_0 = \sqrt{\frac{k}{m}}, \qquad \omega_{\text{nl}} = \sqrt{\frac{|\tilde{\varkappa}V_0|}{m\gamma^2}}, \tag{6.3}$$

where $\tilde{\varkappa} = \varkappa\|\Psi\|^2$. We also introduce

$$\omega_a = \omega_0\sqrt{1 + \left(\frac{\omega_H}{2\omega_0}\right)^2}. \tag{6.4}$$

To construct a solution $\Psi \in \mathcal{P}_\hbar^t(Z(t,\hbar))$ of equation (1.1), (6.1)–(6.2), we are using a phase space trajectory $Z(t,\hbar) = (\vec{P}(t,\hbar), \vec{X}(t,\hbar))$ which obeys (0.5), (0.4).

Using notations (3.8) we have

$$\mathcal{H}(z)=\frac{1}{2m}\vec{P}^2+\frac{m\omega_a^2}{2}(X_1^2+X_2^2)+\frac{m\omega_0^2}{2}X_3^2+\frac{\omega_H}{2}(P_1X_2-P_2X_1); \tag{6.5}$$

$$\mathfrak{H}_z(z)=\mathcal{H}_z(z)=\begin{pmatrix} \frac{1}{m}P_1+\frac{\omega_H}{2}X_2 \\ \frac{1}{m}P_2-\frac{\omega_H}{2}X_1 \\ \frac{1}{m}P_3 \\ -\frac{\omega_H}{2}P_2+m\omega_a^2X_1 \\ \frac{\omega_H}{2}P_1+m\omega_a^2X_2 \\ m\omega_0^2X_3 \end{pmatrix}, \tag{6.6}$$

where $z=(\vec{P},\vec{X})$, $\vec{P}=(P_1,P_2,P_3)$, $\vec{X}=(X_1,X_2,X_3)$, and notations (6.3), (6.4) are used. The matrix of the second derivatives becomes

$$\mathfrak{H}_{zz}(z)=\begin{pmatrix} \mathfrak{H}_{pp}(z) & \mathfrak{H}_{px}(z) \\ \mathfrak{H}_{xp}(z) & \mathfrak{H}_{xx}(z) \end{pmatrix}, \tag{6.7}$$

$$\mathfrak{H}_{pp}(z)=\|\mathfrak{H}_{p_kp_l}(z)\|_{3\times3}=\operatorname{diag}\Big(\frac{1}{m},\frac{1}{m},\frac{1}{m}\Big); \tag{6.8}$$

$$\mathfrak{H}_{xx}(z)=\|\mathfrak{H}_{x_kx_l}(z)\|_{3\times3}=\operatorname{diag}\big(m(\omega_a^2-\eta\omega_{\rm nl}^2),m(\omega_a^2-\eta\omega_{\rm nl}^2),m(\omega_0^2-\eta\omega_{\rm nl}^2)\big); \tag{6.9}$$

$$\mathfrak{H}_{px}(z)=\|\mathfrak{H}_{p_kx_l}(z)\|_{3\times3}=\begin{pmatrix} 0 & \frac{\omega_H}{2} & 0 \\ -\frac{\omega_H}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{6.10}$$

Here $\eta=\operatorname{sign}(\tilde{\varkappa}V_0)$.

Recall, that to find the spectrum corresponding to the Hamiltonian in (1.1) we need only bounded solutions of the Ehrenfest system. The first equation of system (4.5) describes $Z_0(t,\hbar)$, and can be integrated independently from the other equations of the system. The last equation of (4.5) describes the second moments $\Delta_2(t)$ and depends on the solution of the first one. Therefore we start with solving the first equation of (4.5). The simplest stationary solution of it is the zero solution

$$Z_0(\hbar)=\Big(\vec{P}_0(\hbar),\vec{X}_0(\hbar)\Big)^{\intercal}=(0,0,0,0,0,0)^{\intercal}. \tag{6.11}$$

Then the corresponding eigenvalue problem (5.9) has solutions $\Omega_1=\omega_+$, $\Omega_2=\omega_-$, $\Omega_3=\omega_s$, where the Ritz frequencies

$$\omega_+=\sqrt{\omega_a^2-\eta\omega_{\rm nl}^2}+\frac{\omega_H}{2},\quad \omega_-=\sqrt{\omega_a^2-\eta\omega_{\rm nl}^2}-\frac{\omega_H}{2},\quad \omega_{\rm s}=\sqrt{\omega_0^2-\eta\omega_{\rm nl}^2},$$

and the eigenvectors are

$$\begin{aligned} f_1&=\frac{1}{\sqrt{2}}(g_0,ig_0,0,-\frac{i}{g_0},\frac{1}{g_0},0)^{\intercal},\\ f_2&=\frac{1}{\sqrt{2}}(g_0,-ig_0,0,-\frac{i}{g_0},-\frac{1}{g_0},0)^{\intercal},\\ f_3&=(0,0,g_{\rm s},0,0,-\frac{i}{g_{\rm s}})^{\intercal}. \end{aligned} \tag{6.12}$$

Here $g_0=\sqrt{\frac{m}{2}(\omega_++\omega_-)}$, $g_{\rm s}=\sqrt{m\omega_{\rm s}}$. The solutions $a_j(t)$ of (4.7) are found by (5.8) and are normalized by condition (4.8). They form a matrix $A(t)$ (4.13) which we rewrite in the block form

$$A(t)=\begin{pmatrix} B(t) & B^*(t) \\ C(t) & C^*(t) \end{pmatrix}, \tag{6.13}$$

where matrices $B(t)$, $C(t)$ have the following form

$$B(t)=\begin{pmatrix} \frac{g_0e^{i\omega_+t}}{\sqrt{2}} & \frac{g_0e^{i\omega_-t}}{\sqrt{2}} & 0 \\ \frac{ig_0e^{i\omega_+t}}{\sqrt{2}} & \frac{-ig_0e^{i\omega_-t}}{\sqrt{2}} & 0 \\ 0 & 0 & g_{\rm s}e^{i\omega_st} \end{pmatrix}, \quad C(t)=\begin{pmatrix} \frac{-ie^{i\omega_+t}}{\sqrt{2}g_0} & \frac{-ie^{i\omega_-t}}{\sqrt{2}g_0} & 0 \\ \frac{e^{i\omega_+t}}{\sqrt{2}g_0} & \frac{-e^{i\omega_-t}}{\sqrt{2}g_0} & 0 \\ 0 & 0 & \frac{-ie^{i\omega_st}}{g_{\rm s}} \end{pmatrix}.$$

Using (5.25), (5.30), and (4.11) we find a solution of the last equation of system (4.5) in the block form (3.11) in terms of the blocks $B(t)$,$C(t)$ of the matrix $A(t)$ (6.13) as follows

$$\sigma_{xx}(t)=\frac{\hbar}{2}\Big(C(t)D(\nu)C^+(t)+C^*(t)D(\nu)C^\intercal(t)\Big),$$
$$\sigma_{pp}(t)=\frac{\hbar}{2}\Big(B(t)D(\nu)B^+(t)+B^*(t)D(\nu)B^\intercal(t)\Big),$$
$$\sigma_{px}(t)=\frac{\hbar}{2}\Big(B(t)D(\nu)C^+(t)+B^*(t)D(\nu)C^\intercal(t)\Big),$$

where the diagonal matrix $D(\nu)=\mathrm{diag}(\nu_1+1/2,\nu_2+1/2,\nu_3+1/2)$, $\nu_1,\nu_2,\nu_3=\overline{0,\infty}$, and the symbol $(^*)$ denotes the Hermitian conjugate matrix. Matrices σ_{xx}, σ_{pp} are diagonal and their explicit form is as follows

$$\sigma_{xx}(t)=\frac{\hbar}{m}\mathrm{diag}\Big(\frac{\nu_1+\nu_2+1}{\omega_++\omega_-},\frac{\nu_1+\nu_2+1}{\omega_++\omega_-},\frac{2\nu_3+1}{2\omega_s}\Big)$$
$$\sigma_{pp}(t)=\frac{\hbar m}{4}\mathrm{diag}\Big((\omega_++\omega_-)(\nu_1+\nu_2+1),(\omega_++\omega_-)(\nu_1+\nu_2+1),2\omega_s(2\nu_3+1)\Big).$$

The non-zero elements of the matrix $\sigma_{xp}(t)$ are $\sigma_{p_1x_2}(t)=-\sigma_{p_2x_1}=\hbar(\nu_1-\nu_2)/2$.

After substitution (6.12) into (5.10), (5.11) and taking into account that for V defined by (6.2), the vector $V_w(z_0,z_0)=0$, and the only non-zero elements of the 6×6 matrix $V_{ww}(z_0,z_0)$ are $(V_{ww})_{jj}=-V_0/\gamma^2$ for $j=4,5,6$, we obtain the energy spectrum E_ν of the Hamiltonian $\hat{\mathcal{H}}_\varkappa$ (1.1), (6.1)–(6.2)

$$E_\nu=\tilde{\varkappa}V_0+\hbar\left[\Big(\omega_+-\frac{\eta\omega_{\rm nl}^2}{\omega_++\omega_-}\Big)\Big(\nu_1+\frac{1}{2}\Big)+\right.$$
$$\left.+\Big(\omega_--\frac{\eta\omega_{\rm nl}^2}{\omega_++\omega_-}\Big)\Big(\nu_2+\frac{1}{2}\Big)+\Big(\omega_s-\frac{\eta\omega_{\rm nl}^2}{2\omega_{\rm s}}\Big)\Big(\nu_3+\frac{1}{2}\Big)\right]+O(\hbar^{3/2}). \tag{6.14}$$

Note that in the case of zero magnetic field $H=0$, a similar expression for spectrum was obtained in [40].

6.2. One-dimensional case

Consider equation (1.1) with linear operator $\hat{\mathcal{H}}(t)$ in the form

$$\hat{\mathcal{H}}=\frac{\hat{p}^2}{2m}+\frac{k}{2}x^2, \tag{6.15}$$

and the nonlinear operator $\hat{V}(\Psi(t))$ as follows

$$\hat{V}(\Psi(t))\Psi(x,t)=\int_{-\infty}^{+\infty}V(x,y)|\Psi(y,t)|^2dy\Psi(x,t),\quad V(x,y)=V_0\exp\left[-\frac{(x-y)^2}{2\gamma^2}\right]. \tag{6.16}$$

In the absence of a magnetic field ($H=0$), the cyclotron frequency (6.3) is equal to zero ($\omega_H=0$), and thus from (6.4) we find $\omega_a=\omega_0$. Then for the Ritz frequencies we have

$$\omega_+=\omega_-=\omega_{\rm s}=\sqrt{\omega_0^2-\eta\omega_{\rm nl}^2}.$$

The Ehrenfest system with accuracy $O(\hbar^{3/2})$ for operators (6.16) has the form

$$\begin{cases} \dot{p} = -kx, \\ \dot{x} = \dfrac{p}{m}, \end{cases} \tag{6.17}$$

$$\begin{cases} \dot{\sigma}_{xx} = \dfrac{2}{m}\sigma_{xp}, \\ \dot{\sigma}_{xp} = \dfrac{1}{m}\sigma_{pp} - m\omega_{\rm s}^2\sigma_{xx}, \\ \dot{\sigma}_{pp} = -2m\omega_{\rm s}^2\sigma_{xp}. \end{cases} \tag{6.18}$$

As a stationary solution of subsystem (6.17) we take the zero solution

$$Z_0(\hbar) = \Big(P_0(\hbar), X_0(\hbar)\Big)^{\intercal} = (0,0)^{\intercal}, \tag{6.19}$$

In this case matrix $A(t)$ (6.13) of the pseudo-system-in-variations (4.7) is a 2×2-matrix whose scalar blocks $B(t)$ and $C(t)$ satisfy equations

$$\dot{B} = -m\omega_{\rm s}^2 C, \quad \dot{C} = \frac{B}{m}. \tag{6.20}$$

Floquet solutions (6.12) $a(t) = \Big(B(t), C(t)\Big)^{\intercal}$ of the system in variations (6.12) normalized by condition $\langle a, J^{\intercal}a^*\rangle = 2i$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ can be written in the form

$$a(t) = \frac{\exp(i\omega_{\rm s}t)}{\sqrt{m\omega_{\rm s}}} \begin{pmatrix} im\omega_{\rm s} \\ 1 \end{pmatrix}.$$

Then for the energy spectrum E_n of the Hartree-type equation (1.1), (6.15), (6.16) we obtain

$$E_n = \tilde{\varkappa}V_0 + \hbar\Big(\omega_{\rm s} - \frac{\eta\omega_{\rm nl}^2}{2\omega_{\rm s}}\Big)\Big(n + \frac{1}{2}\Big) + O(\hbar^{3/2}). \tag{6.21}$$

Concluding remarks

An approach to the problem of correspondence between classical and quantum models in the nonlinear case has significant differences from the one feasible in linear quantum mechanics. In the linear quantum case, a transition from quantum to classical system in the sense of Ehrenfest requires a certain property of a quantum-mechanical solution, namely the function has to be trajectory-coherent (0.5). A state which does not obey this condition is considered to be essentially quantum, but one which obeys it is near-classical. For the near-classical states the classical dynamics obtained in the limit $\hbar \to 0$ is defined by the classical Hamilton function, and appears to be the same regardless whether the quantum solution is localized (at each moment of time) at a point, on a curve or on a surface. (Exact meaning of localization on a curve or surface is explained e.g. in [2, 3].)

For the Hartree-type equation the situation is different. Classical equations (0.10) (or (3.9)) are valid only for states concentrated at a point in each moment of time. These classical equations are distinct from those obtained in [55–58]. The latter are integro-differential equations which describe dynamics of the n-dimensional manifolds in the $2n$ dimensional phase space. It was shown that for Hartee-type equations an implementation of Born's approach leads to those integro-differential equations for characteristics of a non-local (Vlasov) equation which describes the evolution of the classical density matrix. (Recall that in the linear case, the classical density matrix obeys the local Liouville equation, whose characteristics are trajectories of classical mechanics.) Thus dynamics of point-wise and elongated objects have different equations in the case of Hartree-type models. A rigorous derivation of classical equations describing dynamics of k-dimensional objects ($0 < k < n$) in $2n$-dimensional phase space constitutes a separate open problem.

The Ehrenfest systems (3.5) are subjects of mathematical interest, independent of their quantum origin. Questions similar to those in the linear case, such as about their Poisson structure, and the stability of the solutions (including stability with respect to the nonlinearity parameter $\varkappa$) can be addressed in future study.

In this paper we have shown how the energy spectrum for the Hartree-type equation can be retrieved from a rest-point solution of related Ehrenfest system. Similarly, other quantum characteristics such as quasi-energy spectrum, geometric and adiabatic phases, can be reconstructed

from solutions of corresponding Ehrenfest systems. We will attempt to show that in details in our future publications. Note that in our approach the quantum characteristics can be found without solving the quantum equation. This is particularly valuable and advantageous due to lack of general methods for solving Hartree-type equations.

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Appendix A

Statement A.1. *A solution of equation* (1.1) *with the same Hamiltonian as in* (5.3) *and initial condition* $\Psi(\vec{x},t)|_{t=0} = \psi \in \mathcal{P}^0_\hbar(z_0)$ (2.11) *may be written in the form* (5.6), *where* $\{\varphi_\nu(\vec{x})\}^\infty_{|\nu|=0}$, $\varphi_\nu \in \mathcal{P}^0_\hbar(z_0)$ *is a complete set of stationary trajectory-concentrated states of equation* (5.3), *with corresponding eigenvalues* E_ν, *and* $S[\mathfrak{g}_\psi(t,\hbar)]$ *is defined in* (5.2)

This statement follows from the *nonlinear semiclassical superposition principle*, which we derive first.

Lemma A.1. *Let* $\Big\{\Psi_\nu(\vec{x},t)\Big\}^N_{|\nu|=0}$ *be a set of semiclassically-concentrated mod* $\hbar^{3/2}$ *solutions of equation* (1.1) *with initial conditions* $\Psi_\nu(x,0) = \psi_\nu(\vec{x}) \in \mathcal{P}^0_\hbar(z_0)$. *Then function*

$$\Psi(\vec{x},t) = \exp\Big(\frac{i}{\hbar}S[\mathfrak{g}_\psi(t,\hbar)]\Big)\sum_{|\nu|=0}^{N} C_\nu \exp\Big(-\frac{i}{\hbar}S[\mathfrak{g}_{\psi_\nu}(t,\hbar)]\Big)\Psi_\nu(\vec{x},t) + O(\hbar^{3/2}), \tag{A.1}$$

also is a semiclassically-concentrated mod $\hbar^{3/2}$ *solution of equation* (1.1) *with initial condition* $\Psi(\vec{x},0) = \psi(\vec{x}) = \sum\limits_{|\nu|=0}^{N} C_\nu\psi_\nu(\vec{x}) \in \mathcal{P}^0_\hbar(z_0)$. *Here notation* (5.2) *was used.*

Proof. Consider associated mod $\hbar^{3/2}$ to (1.1) the linearized in $\mathcal{P}^t_\hbar$ Schrödinger equation [36–39]

$$\Big(-i\hbar\frac{\partial}{\partial t} + \widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar))\Big)\Psi = 0, \tag{A.2}$$

$$\widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar)) = \Big\{\mathfrak{H}(z,w) + \frac{\tilde{\varkappa}}{2}\,\mathrm{Sp}\,[V_{ww}(z,w)\Delta_2] + \langle\mathfrak{H}_z(z),\Delta\hat{z}\rangle + \\ + \frac{1}{2}\langle\Delta\hat{z},\mathfrak{H}_{zz}(z)\Delta\hat{z}\rangle\Big\}\Big|_{w=z=Z(t,\hbar)}, \quad \Delta\hat{z} = \hat{z} - Z(t,\hbar). \tag{A.3}$$

Here $\mathfrak{g}_\psi(t,\hbar) = (Z(t,\hbar),\Delta_2)$ is defined in (4.2), vector $\mathfrak{H}_z(z)$ and matrix $\mathfrak{H}_{zz}(z)$ are defined in (3.8). Substitute for the argument of $\widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar))$ (A.3) the expansion $\mathfrak{g}(t,\hbar) = \mathfrak{g}^{(0)}(t,\hbar) + \hbar\mathfrak{g}^{(1)}(t,\hbar)$ (4.3), where $Z^{(0)}(t)$ (4.4) is the principal term of the phase space trajectory. Then with precision $O(\hbar^{3/2})$, we obtain

$$\widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar)) = \mathfrak{H}^{(2)}_\varkappa\Big(\mathfrak{g}_\psi(t,\hbar)\Big) + \Big\langle\mathfrak{H}_z\Big(Z^{(0)}(t)\Big),\Delta\hat{z}_0\Big\rangle + \frac{1}{2}\Big\langle\Delta\hat{z}_0,\mathfrak{H}_{zz}\Big(Z^{(0)}(t)\Big)\Delta\hat{z}_0\Big\rangle, \tag{A.4}$$

where $\Delta\hat{z}_0 = \hat{z} - Z^{(0)}(t)$, and $\mathfrak{H}^{(2)}_\varkappa\Big(\mathfrak{g}_\psi(t,\hbar)\Big)$ is defined by the following equation

$$\mathfrak{H}^{(2)}_\varkappa\Big(\mathfrak{g}_\psi(t,\hbar)\Big) = \Big\{\mathfrak{H}(z,w) + \hbar\langle\mathfrak{H}_w(z),Z^{(1)}(t)\rangle + \frac{\tilde{\varkappa}}{2}\,\mathrm{Sp}\,[V_{ww}(z,w)\Delta^{(0)}_2(t)]\Big\}\Big|_{w=z=Z^{(0)}(t)} \tag{A.5}$$

A solution mod $\hbar^{3/2}$ of the equation (A.2) may be written in the form

$$\Psi\Big(\vec{x},t;\mathfrak{g}_\psi(t,\hbar)\Big) = \exp\Big(\frac{i}{\hbar}S[\mathfrak{g}_\psi(t,\hbar)]\Big)\chi\Big(\vec{x},t,Z^{(0)}(t)\Big), \tag{A.6}$$

and the equation for $\chi\Big(\vec{x},t,Z^{(0)}(t)\Big)$, taking into account (5.2), becomes

$$\Big(-i\hbar\frac{d}{dt}+\langle\dot{\vec{P}}^{(0)}(t),\Delta x_0\rangle+\frac{1}{2}\Big\langle\Delta\hat{z}_0,\mathfrak{H}_{zz}\Big(Z^{(0)}(t)\Big)\Delta\hat{z}_0\Big\rangle\Big)\chi=0, \tag{A.7}$$
$$\frac{d}{dt}=\frac{\partial}{\partial t}+\langle\dot{\vec{X}}^{(0)}(t),\nabla\rangle,\quad \Delta x_0=x-\vec{X}^{(0)}(t).$$

Note that equation (A.7) is defined only by trajectory $Z^{(0)}(t)$, it is linear, and it describes evolution of any initial state from class $\mathcal{P}^0_\hbar(z_0)$ with $z_0=Z^{(0)}(0)$. Thus if the initial state is represented as a linear combination

$$\chi(\vec{x},0,z_0)=\sum_{|\nu|=0}^{N}C_\nu\chi_\nu(\vec{x},0,z_0),\quad \chi_\nu(\vec{x},0,z_0)\in\mathcal{P}^0_\hbar(z_0) \tag{A.8}$$

then

$$\chi\Big(\vec{x},t,Z^{(0)}(t)\Big)=\sum_{|\nu|=0}^{N}C_\nu\chi_\nu\Big(\vec{x},t,Z^{(0)}(t)\Big)+O(\hbar^{3/2}). \tag{A.9}$$

Now, from (A.6) we have $\Psi\Big(\vec{x},0;\mathfrak{g}^0_\psi\Big)=\chi(\vec{x},0,z_0)$, and thus (A.8) can be written as

$$\Psi(\vec{x},0)=\sum_{|\nu|=0}^{N}C_\nu\Psi_\nu(\vec{x},0),\quad \Psi_\nu(\vec{x},0)\in\mathcal{P}^0_\hbar(z_0). \tag{A.10}$$

To complete the proof of the lemma it remains to observe that taking into account (A.6), equation (A.1) is equivalent to (A.9) .

To justify Statement A.1 we take $N=\infty$ and

$$\Psi_\nu(\vec{x},t)=\exp\Big[-\frac{i}{\hbar}E_\nu t\Big]\varphi_\nu(\vec{x},\hbar).$$

Then from (A.1) we obtain (5.6).

Appendix B

Here we derive properties of the trajectory-coherent functions, listed in Section 2.

1. Proof of (2.2). Rewrite the Weyl symbol of the operator $\{\Delta\hat{z}\}^\alpha$ in the form

$$(\Delta z)^\alpha=(\Delta\vec{p})^{\alpha_p}(\Delta\vec{x})^{\alpha_x},\quad(\alpha_p,\alpha_x)=\alpha.$$

Thus, in accordance with (1.5), we obtain the following formula for the mean value $\sigma_\alpha(t,\hbar)$ of the operator $\{\Delta\hat{z}\}^\alpha$

$$\begin{aligned}\sigma_\alpha(t,\hbar) &= \big\langle\Phi|\{\Delta\hat{z}\}^\alpha|\Phi\big\rangle=\frac{1}{(2\pi\hbar)^n}\int\limits_{\mathbb{R}^{3n}}d\vec{x}\,d\vec{y}\,d\vec{p}\Phi^*(\vec{x},t,\hbar)\times\\ &\times\ \exp\Big(\frac{i}{\hbar}\langle\vec{x}-\vec{y},\vec{p}\rangle\Big)[\Delta\vec{p}]^{\alpha_p}\left(\frac{\Delta\vec{x}+\Delta\vec{y}}{2}\right)^{\alpha_x}\Phi(\vec{y},t,\hbar).\end{aligned}$$

Here

$$\Delta\vec{y}=\vec{y}-\vec{X}(t,\hbar).$$

After a change of variables

$$\Delta\vec{x}=\sqrt{\hbar}\vec{\xi},\quad\Delta\vec{y}=\sqrt{\hbar}\vec{\zeta},\quad\Delta\vec{p}=\sqrt{\hbar}\vec{\omega}$$

and using the formula for function $\Phi(\vec{x},t,\hbar)$ from the class $\mathcal{P}^t_\hbar(Z(t,\hbar))$ (2.1), we find

$$\begin{aligned}\sigma_\alpha(t,\hbar) &= \frac{1}{(2\pi\hbar)^n}\hbar^{3n/2}\hbar^{|\alpha|/2}2^{-|\alpha_x|}\int\limits_{\mathbb{R}^{3n}} d\vec{\xi}d\vec{\zeta}d\vec{\omega}\varphi^*(\vec{\xi},t,\hbar)\times\\ &\times \exp\{i\langle\vec{\xi}-\vec{\zeta},\vec{\omega}\rangle\}\vec{\omega}^{\,\alpha_p}(\vec{\xi}+\vec{\zeta})^{\alpha_x}\varphi(\vec{\zeta},t,\hbar) =\\ &= \hbar^{(n+|\alpha|)/2}M_\alpha(t,\hbar),\\ \|\Phi\|^2 &= \hbar^{n/2}\int\limits_{\mathbb{R}^n} d\vec{\xi}\varphi^*(\vec{\xi},t,\hbar)\varphi(\vec{\xi},t,\hbar) = \hbar^{n/2}M_0(t,\hbar).\end{aligned}$$

Recall that the function $\varphi(\vec{\xi},t,\hbar)$ depends on $\sqrt{\hbar}$ regularly, and $M_0(t,\hbar)>0$. Therefore

$$\Delta_\alpha(t,\hbar)=\frac{\sigma_\alpha(t,\hbar)}{\|\Phi\|^2}=\hbar^{|\alpha|/2}\frac{M_\alpha(t,\hbar)}{M_0(t,\hbar)}\leqslant\hbar^{|\alpha|/2}\max_{t\in[0,T]}\frac{M_\alpha(t,\hbar)}{M_0(t,\hbar)}=O\big(\hbar^{|\alpha|/2}\big),$$

Q.E.D.

2. Proof of (2.3) follows from the explicit form of a trajectory-coherent function $\Phi(\vec{x},t,\hbar)\in\mathcal{P}^t_\hbar$ (2.1) and the estimations (2.2).

3. Proof of (2.5). Consider a function $\phi(\vec{x})\in\mathbb{S}$. Then for any function $\Phi(\vec{x},t,\hbar)\in\mathcal{P}^t_\hbar$ the integral

$$\Big\langle\frac{|\Phi(t,\hbar)|^2}{\|\Phi(t,\hbar)\|^2}\Big|\,\phi\Big\rangle=\frac{1}{\|\Phi(t,\hbar)\|^2}\int\limits_{\mathbb{R}^n_x}\phi(\vec{x})|\Phi(\vec{x},t,\hbar)|^2\,d\vec{x}=\frac{1}{\|\varphi(t,\hbar)\|^2}\int\limits_{\mathbb{R}^n_x}\phi(\vec{x})\Big|\varphi\Big(\frac{\Delta\vec{x}}{\sqrt{\hbar}},t\Big)\Big|^2\,d\vec{x}$$

after the change of variables $\vec{\xi}=\Delta\vec{x}/\sqrt{\hbar}$ becomes

$$\big\langle|\Phi(t,\hbar)|^2\big|\,\phi\big\rangle=\frac{\hbar^{n/2}}{\|\varphi(t,\hbar)\|^2}\int\limits_{\mathbb{R}^n_\xi}\phi(\vec{X}(t,\hbar)+\sqrt{\hbar}\vec{\xi})|\varphi(\vec{\xi},t,\hbar)|^2\,d\vec{\xi}.$$

Taking the limit $\hbar\to0$ and using that

$$\|\varphi(t,\hbar)\|^2=\hbar^{n/2}\int\limits_{\mathbb{R}^n_\xi}|\varphi(\vec{\xi},t,\hbar)|^2\,d\vec{\xi},$$

where the function $\varphi(\vec{\xi},t,\hbar)$ depends on $\sqrt{\hbar}$ regularly, we obtain the statement.

Proof of (2.6) is similar to the previous one, if we note that the Fourier image of the function $\Phi(\vec{x},t,\hbar)\in\mathcal{P}^t_\hbar$ may be represented in the form

$$\tilde{\Phi}(\vec{p},t,\hbar)=\exp\Big\{\frac{i}{\hbar}\big[S(t,\hbar)-\langle\vec{p},\vec{X}(t,\hbar)\rangle\big]\Big\}\tilde{\varphi}\Big(\frac{\vec{p}-\vec{P}(t,\hbar)}{\sqrt{\hbar}},t,\hbar\Big),$$

where

$$\tilde{\varphi}(\vec{\omega},t,\hbar)=\frac{1}{(2\pi)^{n/2}}\int\limits_{\mathbb{R}^n_\xi}e^{-i\langle\vec{\omega},\vec{\xi}\rangle}\varphi(\vec{\xi},t,\hbar)d\xi.$$

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